CARNICOM INSTITUTE LEGACY PROJECT

A Release of Internal Original Research Documents

Authored
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Chemistry Vol X

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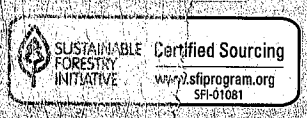


5 SUBJECT

180 Sheets

COLLEGE RULED

Carnicom Institute
Notes

May 2015 –

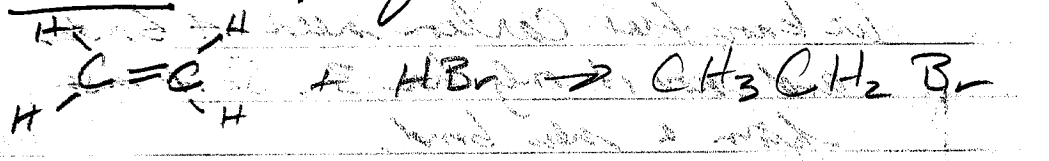
May 28 2015 Thurs

We are moving. The subject is Murray-India Ch 5 and we are towards the tail of the Chapter. Now Sec 5.9.

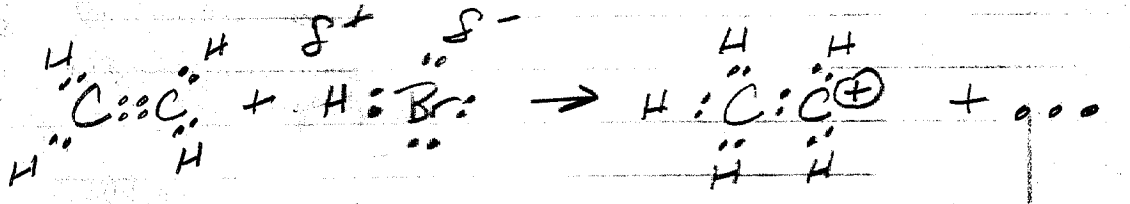
Molecules collide and atoms & bonds reorganize - this is what causes a reaction to occur.

The subject now is that of energy diagrams.

Let's start by understanding more thoroughly the first of two steps of the reaction.



It looks like it's time to start picking up on carbocation as the key element we're seeing. We know that carbocation means a positive C atom.



What do we know here?

1. HBr is polar covalent. $\Delta EN = 2.96 - 2.20 = 0.76$ 1st Step
   the H is just in the polar covalent range.
2. The double bond is a source of electrons & is an electrophile.

So, is this a polar reaction or a radical reaction?

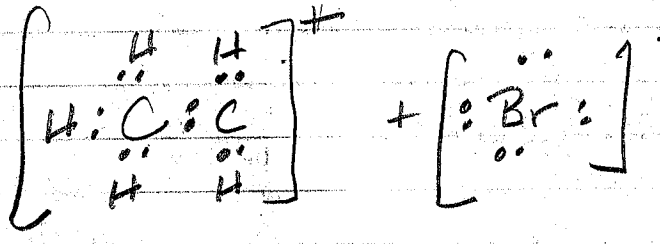
Answer: It is a polar reaction. This means that electrons move asymmetrically. Where do they move to?

We say that they move to the hydrogen of the HBr.

Now if one bond breaks, new bond must form. So what attack to form?

We know that Carbon need 4 bonds and now it only has 3. So it must form a new bond.

Polar reaction are asymmetric b.c. electrons move together to oxygen atom. This leads to



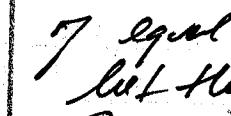
This is the first step.

Intermediate Energy — Br is not bound...

1 C-C = 347
5 C-H = 413
= 2412

2629 - 2412 = +217
Says endothermic, unstable.

The next step is that you now have an electrophile and a nucleophile both of equal & opposite charge so you can tell that they want to combine.
So we will have



Energy:
1 C-C = 1(347)
5 C-H = 5(413)
1 C-Br = 1(363)
Σ = 2775
and 2629 - 2775 = -146 kJ/m
and this is exothermic & more stable.

FC Br / 7 - 1 - 6 = 0

I do see the two detailed steps. I just do not see all the arrow diagram yet.
Let's keep working on this.

Ok yes. I see two electrons move to form the CH bond and I see the two electrons from with the HBr bond staying with the Br.
This actually matches his arrows.

Can I ~~straighten~~ from a ΔH viewpoint?

What do we start with?

1 C=C = 1(614) =
4 C-H 4(413) =
1 H-Br (1)363 =
Σ = 2629 kJ/M

The great you can see why a transition state is unstable & endothermic.

You can also see how a ground state can be more stable, stronger bonds & exothermic.

Each reaction is different but you can now start analyzing reaction from an energy standpoint.

Each reaction has its own energy profile.

Murray gives expected values of reactions - this is very helpful

Most organic reaction have an activation energy of 40 to 150 KJ/mol (remember mole!).

Activation energies < 80 KJ will take place @ a below room temperature

Indeed on Iron Oxides p 96 Ez Chemistry!
There are indeed 2 forms of iron oxides

FeO
and Fe_2O_3 just like ~~it~~ I said

May 29 2015 Friday

Let's re-evaluate our priorities on the final leg of the journey. Now @ Lolo Pass.

1. Advanced Biology Lab
2. Chemistry Lab
3. Seal up Murray - India Clay 5 w/ the final problems.
4. Look @ structure of Vit C & Compare w/ Citrate
5. We also have other virtual Chemistry
6. Can we not prove the formula of iron-oxygen FeO & Fe_2O_3?
   I think that you already have.
7. How about working some organic reaction problems?
8. We have a dissection kit with us!
9. We have the Casio Classpad which is under utilized & the example manual.
10. Math books galore
11. Fun places to go, like Visitor Center @ Lolo
12. Scientific American magazine

$23 \cdot 1E2 = 2300$
$2.3 \cdot 1E3 = 2300$
Raise exp by one. OK.

$23 \cdot 1E{-}2 = .23$
$23 \cdot X = .23$
$X = .1 = 1E{-}1$

$10 \cdot 10^{-2} = .10$
$1 \cdot X = .10$
$X = 10^{-1}$

Fe: Ionization Potentials:

1st	7.9 V
2nd	16.2 V
3rd	30.6 V

$\Delta = 14.4V$

What else has a +3 oxidation state, Al does

1. How do you convert from Volts to Joules?
2. How much iron is in the human body?
3. What is the reaction that changes Fe^{+2} to Fe^{+3} w/ O?

What we have found is that
$1\ eV = 1.602E{-}19J$

So what is an electron Volt?
An electron volt is the energy acquired by an electron when it is accelerated by a potential difference of 1 volt.

So if we have a delta of 14.4V for the 3rd electron removal, it requires

$(14.4V)\ 1.602E{-}19J = 23.07E{-}19J$
$= 2.3E{-}18J$ to strip the 3rd electron from iron.

Now, how much iron is in the human body, esp in the Fe^{+2} form?

$[Fe]^{\emptyset}$ normal valence configuration of iron

$[Fe]^{+2}$ has no valence electrons. but it IS an electrophile

$[:\ddot{O}:]^{\emptyset}$ normal valence configuration of O

$[:\ddot{O}:]^{-2}$ so $Fe:\ddot{O}:$ is FeO

+3 -2
+6 -6

Now, how could you take FeO and change it to Fe_2O_3

1 electron has been removed

$[:\ddot{O}:]^{-2}$

So the question is, what does the Lewis structure for Fe_2O_3 look like?

$[:\ddot{O}:]^{-2}$ Fe $[:\ddot{O}:]^{-2}$ Fe $[:\ddot{O}:]^{-2}$

2 Fe with 3 electrons removed each

This is your idea.

$:\ddot{O}:Fe:\ddot{O}:Fe:\ddot{O}:$

So lets say, hypothetically, that we have one gram of Fe^{+2} in the body.

How many atoms is that?

The molecular molar mass of Fe is 55.85 gms/mol
So w/ one gram we have

$$\frac{1\text{gm}}{55.85\text{gms/mol}} = .0179 \text{ moles.}$$

How many atoms is this?

A mole is 6.02E23 atoms.
So

$$1\text{gm } Fe^{+2} = .0179 \text{ mole}_{Fe^{+2}} \left(6.02E23 \frac{\text{atoms}}{\text{mole}}\right) =$$

$$= 1.078E22 \text{ atoms in one gram of } Fe^{+2}$$

Now, if it take
2.3E-18J to strip the 3rd electron
it then we take

$$(2.3E\text{-}18J)(1.078E22 \text{ atoms}) = 24791 \text{ Joules}$$

to strip off all the 3rd electrons from the entire one gram of iron.

That sure sounds like a lot.

Something seems off here?

Is it possible we do not have the mass here?
But
How about the factor of time... ???
Do you want the instantaneous removal of these electrons or do you want it dispersed over time?
How about over 1 year?
One year = 31536000 sec
So what if we had

$$\frac{24791 \text{ Joules}}{31536000 \text{ sec}} = .0008 \frac{\text{Joules}}{\text{sec}} = .0008 \text{ watts}$$

Continuous.

How much energy does the human body expend during eating, sleeping, running, etc?

What if only 5% of the iron had been changed from the Fe^{+2} to to Fe^{+3} state?

Wallace ID 2yp C-de
83873

Lewis & Clark Trail Crossing Hwy 12

N 46.59550° N
W 114.59986

Iron in the body
Males 4gms
Females 3.5 gms

Body's use 1-1.5 mg per day to replace l.o.s.

Human energy	KJ/min
mowing lawn	30
level walking	17
Walking uphill	32-40
Jogging	40-48

	M	Women
Sitting	9600 KJ/day	8400
Manual work	12,500	9000
Moderate body work	15000	12000
Heavy manual work	19,500	
Extreme Effort	20,500	

X= 9000

Basal metabolism (lying down w/ empty stomach)
7000 KJ per 24 hrs

We should have the info we need now to continue the iron-blood analysis.

Let's return:

ΔV for 2nd to 3rd electron is 14.4 V

We know 1 eV = 1.602E-19 J

So we have (14.4)(1.602E-19 J) = 23.01E-19 J

to pull off the 3rd valence electron of each atom.

We now know that the human body has ~ 3.75 gms of iron in the body. The majority of this is in the hemoglobin and it should primarily be in the Fe+2 state. How many atoms is this?

$\frac{3.75 \text{ gms}}{55.85 \text{ gms/mol}} = .0671 \text{ moles Fe in the body.}$

No atoms = .0671 moles (6.02E23 atoms/mole) = 4.04E22 atoms

Now energy required to strip the 3rd electron from every iron atom in the body is

$4.04E22 \text{ atoms} \left(23.01E-19 \frac{\text{J}}{\text{atom}}\right) \approx 93250 \text{ J}$

Now the next thing we know is that we end up ~ 1.25E-3 gms per day. But this is only how much we end up, not how much is used.

Now assume only 3% of your iron is immediately effected. Therefore .03(93250 J) = 2797.5 J ≈ 2800 J are actually involved.

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Now, how about the question of time...

So now 2800 J of energy are required to strip the 3rd valence electron from 3% by wt blood of the average human body.

Now the question of time. How quickly does this happen?

Instantaneously?

Daily?

Weekly?

Yearly?

How do you know?

We know that we use 1.25E-3 gm per day. At that rate, all iron in the body would be used up in $\frac{3.75 \text{ gms}}{1.25\text{E-}3 \text{ gms}}$ = 3000 days but I suspect you would be dead long before that without replacement & nourishment.

If this were to take place in a day, it would represent $\frac{2800 \text{ J}}{9000 \text{ KJ}}$ = .03% of your energy of today.

P.

The first question concerns the 14.4 V. I do not think you should be using this as the charge is not the same. It take 30.6 V to take the electron off, so this is how much energy needs to be applied, not 14.4 V. 14.4 V will not have the effect, only 30.6 will.
So the energy that corresponds to this is
$(30.6)\ 1.602E-19\,J = 49.02E-19\,J$

We have ~.0671 mole Fe in the body.
No atom = $(.0671\ \text{mole})\ 6.02E23\ \text{atoms/mole}$
$= 4.04E22$ atoms

Energy required w/in body: to ionize 3rd electron
$(4.04E22)(49.02E-19\,J) = 198040\,J$
Now lets say only 3% is ionized:

$.03(198040\,J) = 5941.2\,J$

prorated

How does the wire keeping externally?

$\frac{5941.2\,J}{sec} = \frac{350.5\,K}{min} \cancel{\frac{21030.4\,K}{hour}} =$ day

$= \frac{99.0\,J}{min}$ $\qquad \frac{5.941\,kJ}{sec}$

$= \frac{1.65\,J}{h-}$ $\qquad = .099\,\frac{EJ}{min}$

Lab Leep work on a sense of scale.
Assume 1% of the room is ejected

.01(198040 J) = 1980.4 J = 1.98 KJ

What is this energy if expended over 1 min?
Then it is equivalent to 1.98 KJ / min

= 1.98 KJ / (9600 / 24 / 60) = 1.98 KJ / min = 6.67 KJ / min

= 30% of energy.

What if this energy is expended over 1 day?

1.98 KJ / day / 9000 KJ / day (Sitting) = .02%

Expended in 1 hr:

1.98 KJ / hr / (9000 KJ / 24) = 1.96 / 375 = .5%

Expended over 15 min:

1.98 KJ / 15 min / (9000 / 24 / 4 KJ) = 1.98 KJ / 15 min / 93.75 KJ / 15 min

= 2.11%

Energy Loss Examples

3% / ionization / 15 min
would result in approx x 6 to 3% loss of energy

5% / ionization / 15 min
leads to 10.5% loss of energy.

1% / ionization Level Base Value = 1.98 KJ

Base Value Expended are:

%	9000 KJ/day			
1900%	1 sec	= 1.98 KJ/sec	= 171072 KJ/day	
32%	1 min	= .033 KJ/sec	= 2851.2 KJ/day	
8.20	15 min	= .0083 KJ/sec	717.1 KJ/day	
0.6%	1 hr	= .0006 KJ/sec	51.8 KJ/day	
.02%	1 day	= .0229E-3 KJ/sec	1.98 KJ/day	

But remember if it was 3% then value would be tripled. So the equation is

$$\%\text{ of Sitty Energy} = \frac{1\%\ \text{Base Level Energy in Joules} \cdot \text{Base Multiple} \cdot 100}{\#\text{min} \cdot 60 \cdot \left(\frac{9000\ \text{KJ/day}}{86400}\right)}$$

$$\% = \frac{\text{Base Level (KJ)}}{\#\text{min} \times 60} \cdot \frac{86400}{\text{Sitty KJ/day}} \cdot \text{Base Multiple} \cdot 100$$

$$\%/\text{ionization Level in Blood} = \frac{\text{Base Level (KJ)} \cdot \text{Base Multiple} \cdot 144000}{\#\text{min} \cdot 9000\ \text{KJ/day}} = \frac{\text{Base Multiple} \cdot 31.7}{\#\text{min}}$$

Wallace TD 1 C.A.

May 31 2015 - Sunday

OK, we are on the path toward an oxidation level (ionization) - energy loss, relationship.

Our equation is going to be a function of:

1. The amount of iron in the body
   → No. of moles
   → No. of atoms

2. The amount of energy required to ionize (oxidize) the # of atoms of iron w/ the third valence electron. (total atom number)

3. You need to settle whether ΔE or E in eV is appropriate to use. Remember that Fe++ is already in the body @ the base level.

4. Next we assume a 0th level of the blood that is ionized, ie 1st, 2nd etc. This is a variable.

5. We compute the energy in Joules that is associated w/ that level of ionization (oxidation)

6. Next we need to introduce a rate of ionization (another variable) and compare that to a reference level such as the basal rate and express as a percentage.

So let's go:

1. Iron in the body $\approx$ 3.15 gms

$$= \frac{3.15 \text{ gms}}{55.85 \text{ gms/mole}} \approx .0671 \text{ moles}$$

$$\text{No atoms} = (.0671 \text{ moles})\left(6.02E23 \frac{\text{atoms}}{\text{mole}}\right) = 4.04E22 \text{ atoms}$$

2. Determine the amount of energy required to remove the third valence electron to change Fe^{+2} to Fe^{+3}

$1 eV = 1.602E-19 J$

an electron volt is the energy acquired by an electron when it is accelerated by a potential difference of 1 volt.

3rd Ionization potential for iron is 30.6V

Therefore the energy required to strip (remove) the third valence electron is (iron in Fe^{+2} state) for one atom is $(30.6)(1.602E-19 J) = 49.02E-19 J$.

3. The total amount of energy required to remove all third valence electron from all iron in the body is

$$(49.02E-19 J)(4.04E22 \text{ atoms}) = 198040 J$$

4. The factor now needed to express both the % of Ionization and oxidation is.

$$\text{Rate of Ionization (Oxidation)} = \frac{\%\text{Ionization} \cdot 198040 J}{100 \cdot \text{Unit of Time}}$$

Ie, we have developed a "percentage rate of ionization (oxidation)

Example:

If someone experiences an (Oxidation) of 2% in 15 min of the resting energy loss is

$$\text{Rate} = \frac{2(1980.4)}{15 \text{ min}\left(\frac{60 \text{ sec}}{\text{min}}\right)} = 4.4 \frac{\text{J}}{\text{sec}}$$

Oxidation

Energy Loss

Our usable formula now therefore is:

$$\text{Energy Loss Rate (in } \frac{\text{Joules}}{\text{sec}}) = \frac{\%\text{ Blood (Iron) Oxidation} \cdot 1980.4}{\text{no. of seconds required}}$$

5. Next, what we interested in is a comparison of this rate to the basal metabolism rate.

The basal metabolism rate is 7000 kJ / 24 hr

Therefore the basal rate ≈ ~~7000 kJ~~

$$\text{Basal rate} = \frac{7000000 \text{ J}}{24 \text{ hrs} \cdot 60 \frac{\text{mins}}{\text{hr}} \cdot 60 \frac{\text{sec}}{\text{min}}} \approx 81.02 \frac{\text{J}}{\text{sec}}$$

$$= .081 \frac{\text{kJ}}{\text{sec}}$$

6. Since we are interested in a comparison to a reference rate (ie, in the case, the basal rate) our equation now become:

$$\text{Relative Energy Loss in \% (to basal rate)} = \frac{\text{\% Iron (Blood) Oxidation} \cdot 1980.4\,J \cdot 100}{\text{seconds required} \cdot \frac{81.02\,J}{sec}}$$

$$= \frac{\text{\% Iron Oxidation} \cdot 1.98\,KJ \cdot 100}{\text{sec required} \cdot .081\,\frac{KJ}{sec}}$$

$$= \frac{\text{\% Iron Oxidation} \cdot 1980\,KJ \cdot 1\,sec}{\text{sec required} \cdot .081\,KJ}$$

$$= \frac{\text{\% Iron Oxidation} \cdot 2444.4}{\text{min required} \cdot 60}$$

$$\text{Relative \% Energy Loss relative to Basal Rate} = \frac{\text{\% Iron Oxidation} \cdot 40.7}{\text{min required to Oxidize}} \approx \text{\% Iron Oxidation}$$

$$\text{\% Energy Loss Relative to Basal Rate} = \frac{41 \cdot \text{\% Iron Oxidation}}{\text{min required for Oxidation to occur}}$$

5. Two variables

The equation is

% Energy Loss
Relative to Basal Rate = 40.1 · Iron Oxidation Level
Time Required for Oxidation to Occur (in minutes)

Examples

% Loss	% Iron Oxidation	Time Required (min
4%	1	1
8%	1	5
3%	1	15
8%	2	1
16%	2	5
5%	2	15
12%	3	1
24%	3	5
8%	3	15

Assume time required is a constant & therefore we can propose that energy losses are directly proportional to the oxidation level in the blood. 10% losses are ideal. So we can assume reasonable time periods for the process to occur.

We have a very good graph shaping up.

$1 \leq X \leq 3$ X grid = 6 @ 5
$5 \leq Y \leq$ ~~30~~ 30 Y grid = ~~10~~ 6
$0 \leq Z \leq 25$

& Results

x: % Oxidation	y: Time Required (Min)	z: % Energy Loss	
1	30	1.4%	1 ✓
~~1.2~~	~~30~~	~~1.6~~	
~~1.4~~	~~30~~	~~1.9~~	
1.5	30	2.0%	2 —
2.0	30	2.7%	3 ✓
2.5	30	3.4%	5 —
3.0	30	4.1%	6 —
1.0	20	2.0	2 —
1.5	20	3.0	4 —
2.0	20	4.1	6 —
2.5	20	5.1	7 —
3.0	20	6.1	8 —
1.0	10	4.1	6 —
1.5	10	6.1	8 —
2.0	10	8.1	9 —
2.5	10	10.2	10 —
3.0	10	12.2	11 —
1.0	5	8.1	9 —
1.5	5	12.2	11 —
2.0	5	16.3	12 —
2.5	5	20.3	13 —
3.0	5	24.4	14

Now let's order them in magnitude:

	Energy Loss	Oxidation Level	Time Required
1	1.4	1	30
2	2.0	1.5	30
		1.0	20
3	2.7	2.0	30
4	3.0	1.5	20
5	3.4	2.5	30
6	4.1	2.0	20
		1.0	10
		3.0	30
7	5.1	2.5	20
8	6.1	3.0	20
~~9~~	~~8.1~~	1.5	10
9	8.1	2.0	10
		1.0	5
10	10.2	2.5	10
11	12.2	3.0	10
		1.5	5
12	16.3	2.0	5
13	20.3	2.5	5
14	24.4	3.0	5

We have a very nice graph that we can export if we need to. DPlot should also work.

Let's now to hold the time variable as a constant. Let t = 20 min eg T

% Energy loss = $\frac{40.7 \cdot \text{Iron Oxidation \%}}{t}$

t = 20 min

$\therefore$ % Energy Loss = $\left(\frac{40.7}{20}\right) \cdot$ Iron Oxidation %

Notice in this scenario,
the slope $\cong 2$.
Therefore for a constant 20 min interval
the energy loss is almost twice the
oxidation level.

For a ~~Constant~~ Period of 20 minutes:

Iron Oxidation	% Energy Loss Relative to Basal rate 20 min period
1%	2%
2	4
3	6
4	8
5	10%
6	12
7	14
8	16
9	18
10	20%

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selection of 20 min is a reasonable value.
If we shorten the time too much it will create unreasonable
energy losses and become less realistic for the reaction
to occur to completion.

So here's a question:
How do you simplify the role that time plays?

You're claiming that over a 20 min period, that the energy load is a certain percentage relative to the basal rate.

But why would it vary?
Because the rate of oxidation might vary. But what if we assumed the rate of oxidation was a constant, and if so, what would it be and why?

The goes back to the amount of energy required.

Now the body use about 1.25 mg per day.

This represents $\frac{1.25E-3}{3.759\,mg}$ = .0003 decimal

= .033% of the total amount in the body

Let's recall our problem.

Our generalized equation is

$$\%\ \text{energy loss} = \frac{40.1 \cdot \text{Iron Oxidation }\%}{t_{min}}$$

Solve for t_{min}

$$t_{min} = \frac{40.1\ (.033\%)}{1\%\ \text{energy loss}} = 1.34\ \text{min}.$$

This number is not as reasonable as the one we chose. So look @ the case of a 1% energy loss, 1% oxidation level

$t_{min} = \frac{40.1\ (1\%)}{1\%} = 40.1$ min, This is reasonable.

What we know is that the oxidation level should generally be no more than about 3% & not 10% methemoglobinemia is lethal.

An "average visual point" on our graph is (lower conservative)

~~X=2, Y=10, Z=8.1~~ X=2, Y=20, Z=4.07

So Oxidation level = 2%

Time required ~~time~~ 20 min

% Energy loss = 4.07%

Our choice is a reasonable one.

The graph of your function can be used to identify a reasonable time value.

Assume we want a max oxidation level of 3% for time selection purposes.

Assume we want a modest time level selection. We see 20 min works very well.

So if we want to adopt a optimal reasonable time period in which to make comparisons it is on the order of a 20 min period.

It is true that our focal point of determination appears to rest in the location of

X = 2 Oxidation Level
Y = 20 Time Req. in min
Z = 4.07 Energy Loss

The suggests that a time interval of approximately 20 minutes is reasonable to select selected to form a simplified estimate of the oxidation - energy loss relationship.

Therefore with:

$$\text{Energy loss}^{\%} = \frac{40.1 \cdot \text{Iron oxidation}^{\%}}{\text{time-min}}$$

we may select $t \cong 20$ min.

Therefore

$$\text{Energy loss}^{\%} = \frac{40.1 \cdot \text{Iron Oxidation}^{\%}}{20 \text{ min}}$$

$$\text{Energy Loss}^{\%} = 2.03 \cdot \text{Iron Oxidation}^{\%}$$

Energy Loss Relative to Basal Metabolism $\cong 2 \cdot$ Iron Oxidation Level in % $t = 20$ min

I consider the problem solved w/ a validate model and that a paper can be written from it. I consider the model sufficiently complete

The Oxidation of ~~Blood~~ and Energy loss

to be followed by

The Citrate Prospect.

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May 31 2015 Sunday - cont.

Looking @ our list of May 29 it remains substantially the same. We have however, created an interesting model of the

OK! ~~1. Oxidation of Blood & Energy loss relationship~~.

Which we can now say that we have accomplished!
We also had:

1. Advanced Biology lab
2. Chemistry lab - the real one you have
3. Murray - India Ch 5 final problems
4. Compare Vit C & Citrate structures
5. Our virtual chemistry lab
6. Our dissection kit.
7. Case Classed & manual are here!
8. Math books galore
9. Fun places to go like
   Lol. Para Visitor center ! done!
   Lewis & Clark books galore
   Plant identification
10. Our scientific American magazine
11. What are the structures and reactions that makes FeO change to Fe_2O_3?

$$\overset{2(-2)}{2FeO} + \overset{4(-2)}{2O_2} \overset{?}{\rightarrow} \overset{2(+3)\ 3(-2)}{Fe_2O_3} + 2e^- + 1.5\,O_2$$

$-4 \quad -8$

O: -12

Fe 2

$4(+2)\ 4(-2) \quad 8(-2)$

$4FeO + 4O_2 \rightarrow$

O: -24

Iron lost 4 electrons

Fe: +8

$2 \cdot 3 \cdot (-2)$

O = -12

$4(+3)\ 6(-2) \quad 6(-2)$

$2Fe_2O_3 + 3O_2 + 4e^-$

Fe: +12 O: -24

Iron was oxidized here.

Iron lost 4 electrons

Page 29

We are starting to learn some plants also.
Thus is good.

We have identified a
1. Willow (Salix)
2. Amelanchier (Service berry, saskatoon)
3. Sub alpine fir (Abies) w/ resin blisters!
4. Possibly a Ribes (Currant) species (Ribes hudsonianum is a prospect)
5. On spruce, you see the 4 sided needle @ 10x.
The subalpine fir (and maybe other firs as well) resins have a lot of potential for an insect repellent.
I have mixed it with wide (about 1 to 30 or 50) which is less than ideal but we shall see.
Needle can also apparently be used. I also have ground some green needles in the mortar & pestle.
6. Rhamnus identified. p70
Rhamnus alnifolia - "alder leaved buckthorn".
This is strongly related to the Cascara family
(Rhamnus - Frangula genus name is shared shared - very unusual)
"the all american laxative"
Strong laxative & vomiting properties in the bark.
The berries are POISONOUS

You have successfully balanced the FeO & Fe_2O_3 redox

~~$2FeO + 2O_2 \rightarrow$~~

+2 4(-2) 8(-2) 4(+3) 6(-2) 6(-2) $-4e^-$

$4FeO + 4O_2 \rightarrow 2Fe_2O_3 + 3O_2 + 4e^-$

Iron loses 4 electron in the reaction & is therefore oxidized.

Left	Right
Fe: $4(+2) = +8$	Fe: $4(+3) = +12$
O: $4(-2) = -8$	O: $6(-2) = -12$
$8(-2) = -16$	$6(-2) = -12$
$\Sigma = -24$	$\Sigma = -24$
	$+4e^-$

Fe $+8 = +12 + 4e^-$

O $-24 = -24$.

Now, does the balanced reaction affect your energy equation development at all?

Page 31

Notice that
4 moles of ferrous oxide
produces
only 2 moles of ferrous oxide.

* I suspect this is important.

Indeed, I do believe we have discovered a problem. The oxidation reaction is important.

$$4FeO + 4O_2 \rightarrow 2Fe_2O_3 + 3O_2 + 4e^-$$

The important observation is that 2 moles FeO → 1 mol Fe_2O_3

So back to the problem:

1. Iron in the body is 3.75 gms.
   $= \frac{3.75 \text{ gms}}{55.85 \text{ gms}} = .0671$ Moles primarily in Fe^{+2} form.

2. No Fe^{+2} atoms $= (.0671)(6.02E23 \text{ atoms/mole}) = 4.04E22$ atoms

3. I am actually correct.
   ~~4 atoms~~ molecules of FeO produces 4 electrons,
   I will not change my way here.

Page 32

June 01 2015 – Monday

Let's determine ΔH i.e. endothermic or exothermic for the Fe_2O_3 formation:

$$4FeO + 4O_2 \rightarrow 2Fe_2O_3 + 3O_2 + 4e^-$$

FeO unknown – no services.

O–O = 146

for O:

4(146) = 584

3(146) = 438

?6(146) = 876

1. You need the structure of Fe_2O_3
2. You need the Fe–O
   Fe–Fe bond strengths.

It initially appears like this reaction is exothermic so ΔH may be < 0.

What about Keq?

We can still do this.

MW Fe_2O_3 = 159.6 gm/mol

FeO = 71.8

O_2 = 32.0

So $$Keq = \frac{[159.6]^2 \cdot [32.0]^3}{[32.0]^4 [71.8]^4} =$$

Shift decimal to left, expnent increases towards product
right, " decreases

$K_{sp} = 29.95\,E\text{-}6 \quad = 2.995\,E\text{-}5 = \underline{3.0E\text{-}5}$

The no is, therefore much $<< 1$.
This indicates that the products are not favored and that the reaction is not going to occur quickly at least without a supply of energy. Probably will occur very slowly.

The means that it needs the energy from someplace to take place.

~~But we see a mistake!~~ We use molar concentrations. ~~Not grams. So~~

~~$[\,]^2$~~ No, we are OK still!

See p 226 Ex Chem. You still have the question of whether you are using the equation correctly - Iron oxides, both Fe+2 and Fe+3 are insoluble

Ex Chem p 226 says: Any heterogeneous reaction involving gases do not include the concentration of pure solids. This is most curious...

If this is the case, we simply have $\frac{[\,]}{[\,]^4} = 1.0$ and the is hard to believe.

Iron binding tissues.

In our blood, we do not form iron oxide. Iron oxide is insoluble and this would be dangerous. The organism however does produce iron oxide, & everything says that it is ferric form.

What Zumdahl says on p 1019 is that in g myoglobin

O_2 is directly bonded to Fe^{+2}.
The big question is why it does not oxidize.

Well, Zumdahl answers the question on p 1019-1020 and in doing so has revealed another primary mechanism of damage by the CO.

The answer is that the protein structure within myoglobin (similar to cytochromes) protects & prevents the oxidation from taking place.

He describes the mechanism exactly on p 1020.

Therefore, since the COB readily produces Fe_2O_3 ie ferric iron we know that it is oxidizing the blood. So somehow the COB forms the "oxygen bridge" between the Fe++ ions w/in blood.

June 03 2015 - Wed

On to Countdown now. Leave here on Sat.
Will to happen: hike from Packers Meadow
to Camp Lewis & Clark trail
Also a trip to Powell Range Station.
So two days are taken & I have to pick the best
weather.
We can now regroup on our list of May 31
but now we are confined to two days max.
What are the most desirable?

1. Adv Biology
2. Oxidation Reduction Lab in Chem?
3. A math investigation?
4. The virtual Chem lab?

We are going to look @ oxidation & reduction
in the microchem kit. Very interesting

Page 37

Microchem Kit - Oxidation Reduction #6

This is already very interesting just by looking @ the experiment because by looking @ the activity series of metals you now get entirely the nature of what is happening. You understand oxidation & reduction much better now.

Ez Chem p263 has the activity series.

The most reactive metals are @ the top.

These really would like to gain or electrons

		Std. Reduction Potentials
K	K^+	2.93V 2.92
Ca	Ca^{2+}	2.87 2.90
Na	Na^+	2.71
Mg	Mg^{2+}	2.37
Al	Al^{3+}	1.67
Zn	Zn^{2+}	0.76
Fe	Fe^{2+}	0.44
Sn (Tin)	Sn^{2+}	0.14
Pb	Pb^{2+}	0.13
H 0.0		0
Cu	Cu^{2+}	-.34
Hg	Hg^{2+}	-.79
Ag	Ag^+	-.80
Platinum Pt		-.85?
Au	Au^{3+}	-1.50

Notice Iron is right in the middle. This means it can go either way.

These are generally not reactive.

Nickel is down here somewhere

Reactive w what? ~~well~~, I know.

Page 38

~~... the reaction ...~~

This means that it's highly subject to oxidation. Even metal magnesium

The reaction is set up according to.

	$Cu(NO_3)_2$ (+2, 2(−1))	$Pb(NO_3)_2$ (+2, 2(−1))	$Zn(NO_3)_2$ (+2, 2(−1))
+2 Cu	○	○	○
+2 Pb	◉	○	○
+2 Zn	◉	◉	○

◉ Reaction take place
○ No Reaction take place.

We can now see why & we should be able to predict other sets as well.
According to our chart:
1. Lead is more reactive than copper.
2. Zn is more reactive than copper.
3. Zn is more reactive than lead.

This is why we have these reactions & no others take place.
We have some other metals available. Can we create a different reaction?

Let's look @ nickel and magnesium for example.

Oxidation state of nickel is +2

Now what is more reactive?
We do not have a Std. Red. potential for nickel.
So it is a good example. We do have nickel nitrate in our cleanser. So we should be able to set up

Element	$MgSO_4$	$Cu(NO_3)_2$	$Pb(NO_3)_2$	$Zn(NO_3)_2$
Ni	0	0	0	0

and we should be able to tell where it falls in the spectrum.

For magnesium (which we also have in elemental form) it has an oxidation state of +2. The sulfate ion has an charge of -2 So the formula is $MgSO_4$
We should therefore also be able to set up.

Element	$Ni(NO_3)_2$	$Cu(NO_3)_2$	$Pb(NO_3)_2$	$Zn(NO_3)_2$
Mg				0

Mg is more reactive than Zn
Mg is more reactive than Cu
Mg is more reactive than Pb

makes $Mg(NO_3)_2 + Ni$ $Mg(NO_3)_2 + Cu$ $Mg(NO_3)_2 + Pb$

The should be a great experiment. Page 40
Combine these two metals together.
The was very good work. From this you should be able to tell that magnesium is a highly reactive metal and that nickel is not a very reactive metal (in water). But what about something else like acid?
Mg is also reactive in weak HCl, Nickel is not.

The experiment was successful. Magnesium was oxidized in this reaction and Ni, Cu & Pb were reduced to elemental form.

for the activity you could do w/ aluminum in this picture?

Al is moderately reactive, less than magnesium but more than zinc.

Its oxidation state known is +3.

It is too close to Mg to have a reaction there.

You might be able to get a reaction w/ lead?

$Al(NO_3)_3$???

~~$Al + Pb(NO_3)_2 \rightarrow Al(NO_3)_3$~~

Al w/ lead or copper?

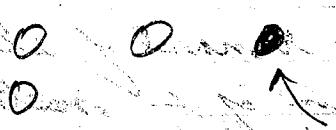
	$Cu(NO_3)_2$	$Pb(NO_3)_2$
Elemental Al	0	0

Al does not likely combine w/ nitrate?

$Al + Cu(NO_3)_2 \rightarrow Al^{3+} + 3e^- + ?$

Cu^{2+} - no metal

Accidental discovery adding $MgSO_4$ solution to clay as a preliminary effort to clean the wells.



$Ni + Pb(NO_3)_2 + MgSO_4 \rightarrow$ reaction ?

$Ni + HCl$

$Mg + HCl$

$Al + Cu(NO_3)_2 + MgSO_4 \rightarrow$ reaction

Produced reactions. This corresponds to:

Al $CuSO_4$? seems likely

$PbSO_4$? seems likely.

You should be able to write the redox reactions for any of these cases now.

Take ~~Cu + Pb~~ $Pb + Cu(NO_3)_2 \rightarrow$?

$Pb + Cu(NO_3)_2 + H_2O \rightarrow Pb + Cu^{2+} + 2NO_3^- + H_2O$

Next, we know that Pb is more reactive than Cu

So we should have oxidation of lead to take place

$Pb + Cu^{2+} \rightarrow Pb^{2+} + 2e^- + Cu$

$Pb^{2+} + 2NO_3^- + Cu \rightarrow Cu + Pb(NO_3)_2$

Pb goes from 0 to +2, Pb is therefore oxidized.

The higher the oxidation no, the higher the level of oxidation, make sense.

to the a pretty cool. You have witnessed some further example by oxidation directly.

This case is the oxidation, a removal of electron from the elemental form of a metal that is higher in the activity series than the metal that is correspondingly reduced.

Thus a good ex present and now I understand the process better than I have before.

Next, the accidental case of sulfate being produced, how would I have known that?

$Ni + Pb(NO_3)_2 + MgSO_4 \rightarrow$? precipitate

$Al + Cu(NO_3)_2 + MgSO_4 \rightarrow$? precipitate

Why did these two react?

$Pb(NO_3)_2 + MgSO_4 \rightarrow Pb^{+2} + 2NO_3^- + Mg^{+2}$

Page 43 lead sulfate ?

$PbSO_4 + Mg(NO_3)_2^- \ldots + Mg^{+2} + 2NO_3^-$

yes insoluble — no soluble

$Al + Cu(NO_3)_2 + MgSO_4 \rightarrow$?

$Al + Cu(NO_3)_2 + MgSO_4 \rightarrow Cu^{2+} + 2NO_3^- + Mg^{2+} + SO_4^{2-} + Al$

$CuSO_4 + Mg(NO_3)_2 + Al^{3+}$ or $Al_2(SO_4)_3$

Soluble? yes — soluble? yes — soluble? yes

So I do not know what happened here?

Back to $Al + Cu(NO_3)_2$

or $Al + MgSO_4$

Aluminum is much more reactive than Copper

So it is indeed subject to oxidation.

Al is NOT more reactive than Mg so this could not have produced a reaction.

Oxidation of Al seem to be probable.

$Al + Cu(NO_3)_2 \rightarrow Al + Cu^{2+} + 2NO_3$ Page 44

$2(+3) + 2(3)(-1) = -6$

$2Al(NO_3)_2 + 3Cu^{2+} + 6e^-$

This seems quite possible

Is $2Al(NO_3)_2$ soluble? Yes. So we would not see it.

Next

$2Al(NO_3)_2 + MgSO_4 \rightarrow Al_2(SO_4)_3 + Mg(NO_3)_2$

soluble would not see it — soluble would not see it

June 05 2015

I am working on a mapping problem and I have an error which is too large discrepancy only by redundant approaches.

Repeat until you find the error.
Found it, I was not aligning the Brunton to the map correctly.

Projector method:

5.5 cm = 5.5(1267) = 6968 m
= 4.33 miles

Bearing = 108°
New project w/ GPS 461-tr2

461-tr1 4.37 miles 104°
461-tr2 4.33 miles 108°

1358

Good. Error is about ~~1000~~ ft.
So we split the difference.

1000 1358 5.9% Ok, but
4.35(5200) = not great.

Split the error portion.
461-tr3
@ 4.34 miles
Bearing 106°

Page 45

error expected:
+/- 670'

This is acceptable.

Or split the error by projector
Bearing = 106°
Distance = 4.35 miles
461-tr4

[redacted]

I have done a molar mass experiment #13 in the micro Chem set. I have acquired completely erroneous results and I have no idea why. The solution did not turn pink nearly as quickly as it should have and I had to dilute it by a factor of 5. My results of 3.6 adjusted by the factor of 166/52.1 =

First, I learn that the litmus paper is totally different than I did not use it any way. But I need a replacement.
The phenopthalein test indicates to just fine. It turns pink upon alkaline. It still works.
So why did the experiment fail?

In the form of salt, a level teaspoon weighed 6.29 gms.
This already an error of 20%.

Now we do not want to use our chemicals up
So we are going to use 0.2 gms instead of 1.0 gms.
The solute dissolves by a factor of 5
Stirred & dissolved

Page 46

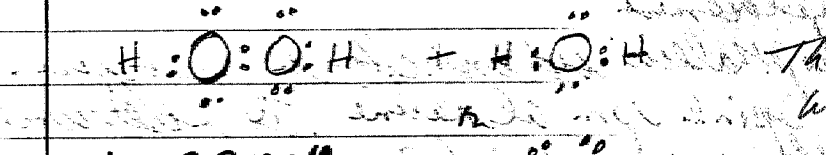
Take 2 ml of the 4 titrate.
13 drops?

One proportion.

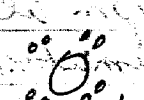
We noted in the first trial that it was taking an inordinate amount of ~~NaOH~~ NH_4OH to counteract the KHP. This was our first indicator of a problem and so we chose to obtain a fresh bottle of NH_4OH.

The should not have been needed. Everything indicates that the NH_4OH may not be as strong as it once was.

Question – Can NH_4OH ever weaken with age? What would be the mechanism for this? We know that H_2O_2 does...

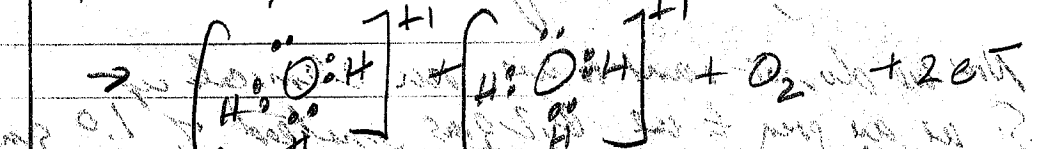


Hydrogens separate, make H_3O^+



and O_2 leaves the solution.

Does NH_4OH weaken over time?



FC = 6 – 3 – 2 = (+1)

Ammonium is NH_4^+

Ammonia is NH_3

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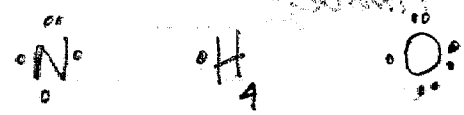
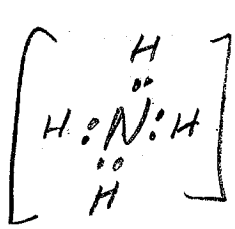
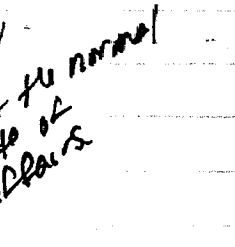


FC = 5 – 3 – 2 = 0

NH_4OH weakly dissociates into ions

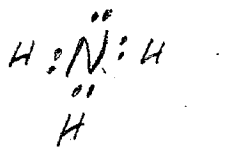
Structure is



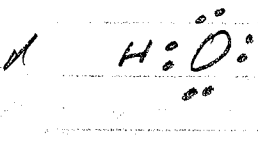


FC: $5-4-0=+1$ $\quad$ FC: $6-1-6=-1$

Wants to transform to



and



which is ammonia + water

which is no longer ammonium hydroxide.

I believe that is the solution to my problem w/ the experiment. Ammonium hydroxide has partially degraded to ammonia and water.

This is also why the hydroxide ion is diminished in number & why it is taking more of the "weakened ammonium hydroxide" to have an effect.

Good work. Where do you get ammonium hydroxide?

June 10 2015 - Back in Wallace ID,

OK, let's get our plans in order. Lab only for now.

[redacted]

In the lab we have some instruments coming.
But for now, we focus in some basics.

You can always write papers of course.
But for now I am interested in some basics
of the lipids.

1. Boiling Point
2. Freezing Point
3. Distillation
4. Soaps
5. Polymerization repeat?
6. Molecular Weight Determination

} do we have purity?

6. Colvatile fats
7. Bacteria tests + strips?

There are now about 6 types of oil in the freezer
including CBD Lipids.

1550 ~~Frozen~~ Liquid Page 50

~~Flaxseed -24c~~ 1.480 ~~Almond -8°C~~
1.458 Olive -6°C ~~Hemp -24c~~ -8°C
~~Vegetable (usually soy) -16c~~ CBD
~~1.465~~ ~~Sesame -6°C~~ Flaxseed -24°C
1.474 Sunflower -17°C Vegetable (usually soy) -16°C
Sesame -6°C
Sunflower -17°C

~~So how can you get the results that you have?~~
OK now. They were not frozen

CDB Lqd ~~Lsteth~~ Distillati Attempt;
1/2 Mix w/ Water in ~20 ml test tube.
Seal or broke. 3 clamps.

C

1855 31.7° Something is already happening.
Could be acetone.

1015 90.7 Reaching top of tube. Aluminum
jackets needed to build sufficient ~~heat~~
Tubing may be suffering damage

1025 93° Something is boiling off. It destroyed
tubing.

It all boiled off @ this temperature
This indicates that it is fairly pure

But you also know that you had 1/2 water
in there so this means that it mixed
with water under sufficient heat

After cooling entirely, the residue in the
beaker has definitely produced a greasy
material.

It is like grease in a frying pan.

Page 51

Mini

Repeat Distillation Experiment.

1930 29.3°C Top Thermometer
40°C Sand Thermometer

1941 33.3 Top
93°C First Bubbles form (bottom)
This does seem to be the boiling point.

1955 31.9°C
105°C Low key steady stream boiling.
Since the bubbles seem to be coming from the bottom, how do you know that it is not the water that is boiling?

We have now brought it to a brisk boil. and will now cool off. Will it separate?

Upon Cooling, separation did indeed occur. However, the water portion is now cloudy, so something mixed in slightly w/ the water. No detectable volume difference.

Start again.

The Freezing Oils Experiment

Time
1550 – 2010

	Freezing	Viscous	Liquid
-6°C	Olive	-24°C Flaxseed	CDB
	Vegetable	-24°C Linseed	Hemp -27°
-17°C	Safflower		Almond -10 to -2
-6°C	Sesame		
	Super Omega 3 (Fish Oil)		

Only remainders are hemp & CDB

Overnight
Almond Freezes
Flaxseed Freezes
Linseed Freezes

Some observations

1. When you heat it high enough it melts an emulsion
2. When you cool it off the emulsion it makes a grease.

2035 Bottom 60°C
Top 29.9°C

2110 @
Top 89.9 ! ~90°C

Very clear separation taking place here
Perfect distillation apparatus constructed.

Two different forms are coming out.
In dense thick form almost one can
watch that I mixed i.e. that does not count.

Hemp freezing point allow to be -27 to -28°C
Hemp oil has a refraction index of 1.477

Jan 11 2015

We are indeed learning quite a lot about the general properties of the CDB Lipids

1. We have a further separation by heating to 93°C (thin-distillation)

2. Refractive index is unusual @ 1.487

3. Boiling point appears to be approx 93°C

4. Freezing point appears to be < -28°C
Regression Prediction = ~~-43°C~~ -45°C

revised

We have recorded the data & the correlation between Index of Refraction & Iodine number.

Now we wish to ~~con~~ investigate a relationship between IOR and freezing points, boiling pt

---

It seems to me that there is a good chance of a relationship w/ IOR & M.P. & Boiling pt
Will now pursue on original IOR notes

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Yes, there is indeed a fairly good relationship.
From the relationship developed

Freezing Point = 2509.1 - 1716.5 (Index of Refract)

and with an index of refraction of 1.467
and observed liquidity up to -24°C
We have a
Predicted freezing point of COB Lipids
as -43°C Am revising

Now lets go for direct freezing point
Direct COB Sample

1420	27.5°C	Heat on 4
1425	37°C	
1431	56°C	
1435	66°C	Heat on 3 No activity
1437	71°C	
1440	81	
1445	90	
1450	93	No Activity.
1455	96	
1500	97.5	
1505	100.0	
1510	100.5	No activity
1515	103	Raise to 3 1/2
1525	106.5	
1530	108	
1535	109	
1540	109	Raise to 3 3/4
1600	112	
1615	118	Raise to 4
1640	123	Raise to 4 1/2
1655	125.5	Raise to 5
1700	128.5	

1610 131.0°C
=266°F

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COB Login Freezing Point Estimate

For sorting to revise the curve.

I will take COB estimated freezing point as
-40 instead of -35
This remains a Conservative estimate.

1.407

r=.81

Freezing temp = 2602.3 - 1780.3 (Index of refra

This leads to a predicted freezing point of -45

3.05 gms acetone

3.68 ~~3.60~~ w/ oil

Yes 342.3

excellent

The molecular mass idea
Colligative Properties.

$\Delta T_b = K_b \cdot m$ ← molality — m = molality

↑ temp increase because of solute

↑ boiling pt elevation constant for water

molality = # moles / kg. of solvent

also called "molal"

Example. Can we solve for the molecular mass of sugar.
Here we place 50 grams sugar in 117 grms of water
So

$$\text{Molality} = \frac{.146 \text{ moles}}{.117 \text{ kg}} = 1.25 \text{ molal}$$

This is not our problem, as do not know the # of moles of sugar from Thin Layer.

Molecular weight = grams solute (composition unknown) / moles of solute.

already equation but previous section

So moles of solute = grams solute / molecular weight of solute

So molality = grams solute / (molecular weight of solute · kg of solvent)

So

$\Delta T_b = K_b \cdot \frac{\text{grams solute}}{\text{molecular wt of solute} \cdot \text{kg of solvent}}$

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or Molecular wt of solute = $\frac{K_b \cdot \text{grams solute}}{\Delta T_b \cdot \text{kg of solvent}}$

yes this is correct!!

Sample 3.05 gms a
0.63 gms oil

~~Molecular wgt determination~~

Acetone boils @ 56.2°C Control

@ #3

1810 39°C
1815 44°
1817 48° Bubbles Steady to Fast drop to 2
1818 57° Drop to 1.5 Light bubbles
1819 53° Steady vigorous bubbles
1819 54° Definitely a full boil.
Thermometer accurately boiling
Turn off heat.
Now for Sample
No

1825 44° Bubbles already visible

Appear to be about ~~57°C~~ 57.6°C

Any thing slowly reaches a max temperature
Record this maximum.
Don't worry about intermediate stage

Oil does appear to be soluble in acetone

Acetone again

1835	52°	bubbles start
1838	56°	Intermittent boiling
	56.8	best estimate

Use 56? 56.2

Let's try it. Use 56.2 Acetone
57.6 Oil Mix
$K_b = 1.67$

$$\frac{1.67(0.63)}{1.4(.00305)}$$

$$= 246.4 \frac{grams}{mole}$$ Very interesting. Reasonable number.

Our proposed ACD structure is 170.2 $C_8H_{10}O_4$

$$\Delta MW = -K_b \cdot \frac{grams\ solute}{\Delta T_b^2 \cdot kg\ of\ solvent} \Delta(\Delta T_b)$$

$$= \frac{-1.67(.63)}{(1.4)^2(.00305)} (.5) = \underline{87}$$

Range = 159 to 333 ~~that is pretty wide.~~

Page 60

3.80 acetone
5.00 to 2nd
w/ sample

Repeat

1935 41° sand on 2
1940 46°
1943 56 sand
1945 63°
1948 70°
1951 77
1955 83 on 2.5

2000 56.1 Sand

Method is to get it hot.
Covered w/ Foil.
Then punch thru quickly &
take measurement & get out.
~~If dem~~ IC volume decrease it was
already hot.

59.8 sample

$$MW = \frac{(1.67)\,1.28\,gms}{3.7^{\circ}C\,(.0038k)} = \underline{\underline{152.0}}\ MW$$

This should be a better measurement.
Predicted structure is ITO

Good work

error est. is $\frac{-1.67(1.28)}{(3.7)^2(.0030)}(\emptyset.3) = \underline{\underline{12}}$

Very good work here. Range 140 to 164

Page 61

4.81 acetone

Repeat & you may have a handle on MW.

MW of Sunflower oil = 876
" Palm Oil 810 - 855
THC vs Hemp Oil 314.

OK, let's do it again.

Chemicalize.org has some structural properties

OpenMolecules.org

Molinspiration.com

Again Acetone 4.97

~~4.4~~ Acetone 4.55 56.2
Sample 5.38 ~~54.7~~ 57.8

$$MW = \frac{1.67(.83)}{1.8(.00455)} = 169.2$$

Not Bad.

169.2
× 152.0
= 160.6 = 161 and avg error = $\frac{28+12}{2}$ = 20

Error Analysis on 2nd run:

$$\frac{-1.67(.83)(\phi.3)}{1.8^2 .00455} = 28^\circ$$

So the range is from 141 to 181
with expected error of 20
And a mean of 161

Page 63

Jun 12 Molecular Weight ~~Third Trial~~

~~3.93~~ ~~3.90~~ 3.91

~~5.10~~ ~~56.2°~~

3.79 56.2

5.20

60.0 N

~~60.3~~

$\frac{1.67(1.41)}{3.8\,(.00379)} = 163.5$

$\text{Error} = \frac{1.67(1.41)\,.3}{3.8^2\,(.00379)} = 12.9 = 13$

Si Average are 152

169

163.5

$\bar{X} = 161.5$

$\sigma = 12$

$+20$

$+13$

$\sigma = 15$

Si range is 146 to 176.

Mean is 162

σ is 15

$= 9.9 \pm 26$ Daltons

Pretty Close

Page 64

Jun 13-2015

Today.

Lab one test on boiling point - Molecular weight

2. Get a lab solution running + record the signal pastical document.

I have made the solution. The pH is too high but we will see how it works. Now @ 12.5
1100 Jun 13 2015

~~3.69~~ ~~3.95~~ 56.2
4.94 60.1

3.94
5.20

Error = $\frac{1.67(1.20)(0.3)}{3.9^2(.00394)}$ =

Most Stable Supports Used

$MW = \frac{1.67(1.20)}{(3.9).00394} = 136.9 = 137$

This certainly is a low study.

Page 65

Now are values are 152 Errors 12
169 28
161 13
137 10
$\bar{X} = \frac{155}{}$ $\sigma \Sigma = 16$

CRC = 1.80 not 1.67
1.80 (155) = 167.1 preferred value
1.67

$\therefore$ range $\approx$ 140 to 170

Molecular Weight Determination

[redacted]

~~3.3~~

3.88

5.24

~~590~~

60.3

Error = $\frac{1.67(1.36)(.3)}{4.1^2(.00388)}$ = 10.4

$MW = \frac{1.67(1.36)}{4.1(.00388)} = 143$

Error

So now we have

2.10	152	$\times(1/12) = 12.67$
1	169	$\times(1/20) = 6.04$
2.05	161	$\times(1/13) = 12.38$
2.27	137	$\times(1/10) = 13.70$
2.36	143	$\times(1/10) = 14.30$

$X = 152.4 = 154$

Lipids are medium sized, This is a middle size biomolecule

Weighted Average by Error

So $\bar{X}_{wt} = \frac{12.67 + 6.04 + 12.38 + 13.70 + 14.30}{1/12 + 1/20 + 1/13 + 1/10 + 1/10} = \frac{59.09}{.473}$

$= 9.04E25$ Daltons

Weighted by error

$MW\ X_w = \frac{1466.72}{2.1 + 1 + 2.05 + 2.27 + 2.36} = 149.97 = 150$

$\sigma_{avg} = 15$ So range is 135 – 165

1 Dalton = 1.66E-24gm

June 14 2015 Sunday

1. ~~There is~~ now an estimate on the molecular weight of the lipid. This is important. The molecular is settling in @ ~ 150 with σ = 15

2. It is interesting that this corresponds fairly well (170) with my predicted structure. We are after the little equipment.

3. You also have at least a first ~~estimate~~ of the freezing point (based upon an IOR - freezing point correlative model) joined w/ observations. @ -45°C

4. I would like to pursue smoke point next

5. Then I would like to try test strips again

6. The polymer idea is very interesting.

7. The lile solution is in place for the next. Starting date was June 13 @ pH 12.5
Today June 14 is pH 12.2

8. You have incredible books on hand now.

9. There seems to be alternative interpretation of Daltons. No, it is all OK ~~now~~ now. The mass of a Dalton is not the same thing as a dalton. 1 dalton = 1 gram per mole!

page 67

10. From Carol Gore classroom she states lipids are approx 2% up to 30% of the total mass (?) of a bacterial cell. She would place our best estimate of bacterial mass @ 15% (or 155 gms/mol) = 2325 gm/mol.

11. The soap idea is also interesting.

On Daltons, the only definition of the dalton is one gram per mole. (It is a unit of mass per mole. There is not the same thing as mass. The actual mass of a dalton is 1.66E-27 kg which is 1/12 the wgt of one carbon atom. So do not get this mixed up. So when we use molecules we are using EDA for example.

We have set up a polymer experiment (Fat (Liquid), Enzymes & Sugar

OK, lets try smoke point. We could use heat also? Record.

Flaxseed ~ 260°F = 127°C
COB ~ ~~90°~~ = ~~88°~~ Page 68
COB 185°F = 85°C Smoke Point

S: 10R 1.407
Smoke Point 85C
Freezy Point -45°C (est)
Molecular Wgt ~ 160

Tentative structural formula which meets MW observations reasonably well

[redacted]

We originally wanted on June 10

1. Boiling Point (oils do not boil except at high temperatures)
2. Freezing Point
3. Distillation — we have done quite well on the list.
4. Soaps
5. Polymerization — what reaction is:
6. Edvotek Class
7. Bacteria test strips
8. Osmosis?

1. Edvotek Class
2. Test strips repeated
3. Osmosis method of molecular weight determination
4. Heat lipids to look @.
5. Mill Lake & oven.

Osmotic Pressure Role Constant

Osmotic Pressure Relationship
for Molecular Wgt Determination

$\Pi = \frac{g\,R\,T}{MW \cdot V}$

Is this an Constant that is available? We had a temperature Const

g = mass of the solute in gms
V = Volume of solution in liters
MW = Molecular Wgt of the solute
R = the gas Constant = .082 $\frac{\text{atm-liter}}{°K - \text{mole}}$
T is absolute temperature
Π = the osmotic pressure in atmosphere

Also Π = Molarity · R · T

~~Learn to use Pen Test~~

No

Molarity = $\frac{g}{M \cdot V}$ or MW = $\frac{g}{\text{Molarity} \cdot V}$ Is this true

Check w/ an example from my biophysics book:

MW = $\frac{69.3 \text{ gms}}{\text{mole}}$

Page 70

Does $\frac{g}{M \cdot V} \stackrel{?}{=}$ Molarity yes = $\frac{\text{moles}}{\text{Liter}} \cdot \frac{\text{grams}}{\text{per unit Volume}}$

= 0.5 Molarity

g 8gms Carbon in 1 liter
= 8gms / 16 gms/mole * 1 liter

Osmosis experiments

Cellophane is not permeable by observation.
Some people say it is, others (I) say it is not.
My observation and all says that it is not.

10.1 to 13.7 gms of sugar water,
So this worked great.

The thistle tube has moved from 0.4 to 0.55
It is moving but very slowly.

You have the following on order.

Ringstand & Rod — Frey Scientific
2 Clamps
Dialysis Tubing 1 3/4 (= 3 1/2)
50 13x100 Test Tubes
~~Thistle Tube~~
~~Thermometer~~

~~Osmosis is going to work~~ You just need the
~~better membrane material~~

Page 71

The Osmosis approach

g 5 gms
1 mole

Mole mass = $\frac{\text{grams of solute (known)}}{\text{No. of moles of solute (unknown)}}$

moles
mass ÷
5 gms/mole

We need to find the molarity using the relation

$\pi = MRT$ ← Constant
π ← sometimes measured.
M ← Molarity
T ← Known Temperature °K

We can't do this directly so how do we determine it.

Solve for $M = \frac{\pi}{RT}$ ← we need this.

The osmotic pressure is simply the difference in height that occurs!
Apparently it does not matter about the volume or dimension of the tube!
Maybe Not!

1.80(655) = 1.67
1.67

It is very interesting to me that CRC lists the freezing point elevation Constant of acetone as 1.80 not 1.67.

vs 1.71 is pretty darn close.

Why the difference?

Your source was wikipedia. All Wikipedia is constantly lower.

Page 72

Wikipedia or based upon 1941 to 1970. reference.

Jun 15 2015

PH of bile solution is: 12.2. No Change today
Thistle tube has risen very slowly. Dialysis tubing is required. The bladder version eventually is diffusing out of the bag back into the surrounding solution.

Back to osmotic pressure measurement.
One source, actually two now, say that ΔL IS the osmotic pressure.

From Pavia Intro to Laboratory Techniques (an old book)
in general, the boiling point increases as the molecular weight increases

Acetone has a molecular weight of 58.1 gm/mol
Xylene has a molecular mass of 106.2
Isopropanol is 60.1

The bonds of unsaturated oils are easily broken, there is a reason that unsaturated oils boil @ lower temperatures. The smoke point always come before the boiling point.

Amazing discoveries in the CRC Handbook. What a wealth of info assembled in one place. Boiling point elevation Constants are different!

You are discovering today that you have some very good books.

PAGE 73

Fractional distillation is the same principle as gas Chromatography. How about that?

Jun 15 2015

Ok, what a day now and out next 3 days?

1. Gahotek kits
2. Test strips
3. Osmosis kit
4. Biology kit

or!

5. Vacuum distillation?
Coming up!

Well fractional distillation was a great idea but it did not work.

Why?
Because your vacuum pump can not sustain a vacuum because it overheats. Good try.

Jun 16 2015

pH of bulk today is ~ 12.4
No real change yet.
It is possible that the two alkaline
Should have been @ ~~7.5 to 8~~ 9 to 9.5

How about we get a second generation org.?
11.9 still too high. Do not need much NaOH.

Our list now is:
yes! ok ~~1. Do we want to try Osmosis again w/ clamp & stand?~~
2. Test strips
3. Evolve
4. Biology kit
5. Still working on the osmotic pressure extractor.

Test strips are in motion.
We know again now that the COB can use
Citrate as a nutrient source.

There is a ferric citrate and it is involved
in ferric siderophore
Found in Google Books:
"Transition Metal in Microbial Metabolism"

Ferric citrate transport has been well
documented in gram - nitrate bacteria.

Jun 16 2015 1700

Culture / Citrate Trial
We know the CDB uses and Citrate
(cut back w/ Fe^{+3} ions)

Tests:

30 ~~40~~ ml of sodium citrate in all

Variables..
Fe^{+2}
Citric acid
H_2O_2
Sugar
Water
Lemon Juice

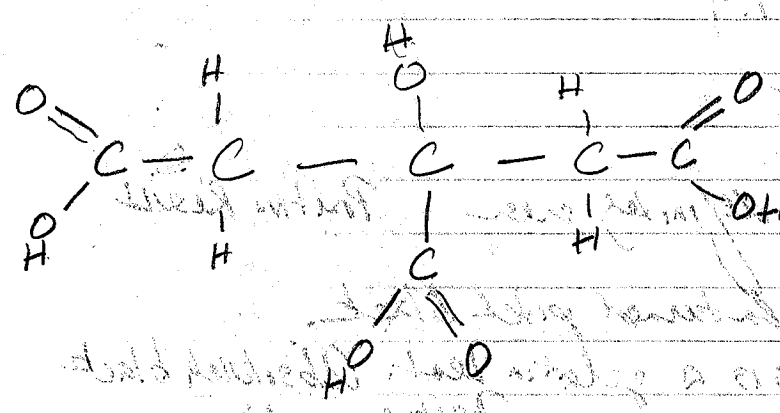
30 ml Sod. Citrate
4 drops CDB
.10 gms Fe^{+2}
Lemon Juice is 6 drops
H_2O_2 is 6 drops
Citric Acid is 0.25 grams
Sugar is 0.25 gms

Water, Sugar, Iron
Citrate +

1. Citrate + CDB + ~~Fe+2~~
2. Citrate + CDB + Lemon Juice
3. Citrate + CDB + Fe +2 + H_2O_2
4. Citrate + CDB + Fe+2
5. Citrate + CDB + Fe+2 + Comm. C[illegible]
6. Citrate + CDB + Fe+2 + Comm. Vit C
7. CDB + Sugar + Water + Fe+2
8. CDB + Water + Sugar + Fe+2 + [illegible]

It looks like you get to apply your studies of acid base Chemistry to citric acid.

Buffers consist of a weak acid and a conjugate base
or
a weak base and a conjugate acid.



Then on citric acid. Let's start to learn what we applied.

$C_6H_8O_7$

June 17 2015

The instruments are scheduled & arrive. Let's see what happens

(1) pH
#1: 12.2
#2: 11.9

API 20E

(2) CIT is definitely green Positive Result

GEL has turned pitch black
This is a gelatin test. Absolutely black.
positive result

(3) Thistle tube - is actually doppy!
The opposite what we expected!

(4) Culture:
1 Clear
2 Green
3 Green
4. Green
5. Green
6. Brown + little of any growth
7. Rust - clear growth
8. High level of growth.

Gelatinase is a proteolytic enzyme that allows an organism to hydrolyze gelatin into its amino compounds

derived from collagen - gelatin

Factors By:

Blood 1. Iron
2. Lipids, poly unsaturated, oxidation, polymerization
Energy 3. Citrate - (sole carbon source or not)
Protein Degr 4. Gelatinase
5. Gram negative
6. Heat & Acid Tolerant

Citrate medium
Sodium citrate
ammonium phosphate
Thousand ammonium sulphate

#9 will be

.25gms 1. Sod Cobalt
.10gms 2. Fe+2
6 drops 3 Peroxide
~~4.~~
.25gms 4. Ammonia sulphate
5. 6. H_2O
6. CDB
4 drops

#10 will be

.25gms 1. Sugar
2. Fe+2
3. Peroxide
4 Ammonia Sulphate
5. H_2O
6. CDB

June 19 2015

Start on Jun 13 5-6 days now

(1) pH #1 is 12.75
#2 is 11.0

This is not so good so we are not so sure that fatty acids are being created.

(2) Possible polymer growth in your culture

(3) Culture series of extract, esp w/ Vit C?

(4) Osmosis test fails need proper material on the 22nd.

(5) We have a good evaporator oven now.

(6) You can start evaluating spectra soon.

June 19 2015

Start on Jun 13 5-6 days now

(1) pH #1 is 12.75
#2 is 11.0

The r not so good so we are not so sure that fatty acids are being created.

(2) Possible polymer growth in your culture

(3) Culture serves as substrate, esp w/ Vit C?

(4) Osmosis test jars need proper material on Fig 22.

(5) We have a good evaporate over now.

(6) you can start evaluating spectra soon.

Page 82

We now have the first reliable spectrum of COB lipids. Let begin first functional analysis.

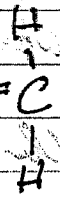
Our first major group appears 3150-6 2800

3100 - 2500 is Carboxylic Acid
Looks like a strong candidate

Now within this range:

~~3120~~ 3022
IR Spec 3020 is Alkene C=H
This is also strong

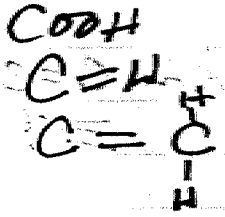
Next is 2967
IR Spec gives 2975 as alkene C-C



Next is 2923
IR Spec gives 2925 as Alkane C-H

Next: 2868
IR Spec gives 2870 as Alkane (methyl) C-H

So we have



C-H

Next is 2734
IR Spec 2720 aldehydes

Koji has CHO
N-CH_3

2734 is aliphatic aldehydes
a possibly CH stretch from Meloan
which is a CH Typ chart

Avram also has R-CHO
which is [illegible] both aliphatic and aromatic.

This is a pretty good choice

Now 1716
~~Very interesting~~. IR Spec has ketones from 1715-1720, This is a very good match
C=O so it is a carbonyl group.
It also says saturated or a 6 membered ring
Fits well.

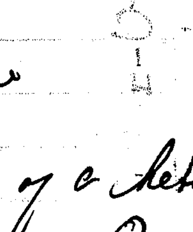
But Chem toolboxes also has ketone C=C stretch !

or an aromatic ketone

Page 84

What is the definition of a ketone.

A ketone is only



Lots of things are ketones
See Chem toolbox

Skipped Page by Accident

1614 Alkenes & Arenes both appear to be strong candidates.

One of your questions does C=O always have a double bond? Good to answer will be no. But a Carbonyl does have a double bond.

Functional groups are listed very well on page 67 on McMurray India and the Chem Toolbox has a wonderful presentation

Our partitioned IR chart shows what is happening w.r.t. single & double bonds.
We see that the region of mid IR are very revealing.

The aldehydes @ 2720 . . . .

The section should move ahead to "Skip To Here Section" (~6 pages)

June 21 2015

As usual, a lot is going on.

OK 1. ~~The pH of the lute solutions~~ this time did not ~~decrease~~. Too much NaOH, too little lute likely. ~~Will need to~~ forge ahead. [BUT IT WORKED PERFECTLY!]

2. We need spectra of filament (EPA preferred) & CDB today (whole).

3. It would be of interest to compare the two oils again. (feature)

4. Can we digest the proteins somehow?

5. Can we digest the filaments somehow?

OK 6. ~~Look under scope at Canning culture - Same as normal~~

7 ~~Replenish~~ & evaluate petri cultures?

8. ~~Base tube has been repaired. It came up~~ ~~some with~~ semblance of the thistle tube!

I have produced a very decent volume of lignin today. It went like clockwork. I now have plenty to work with.

The osmosis tube is also working for the first time! The tube IS rising!

Today we would like to follow 3 spectra

1. COB Lipids – old & new sample
2. COB whole
3. ERA thru. filament & one other.
4. Your program on a flash drive.

on ERA filament

lets scan for 4000 – 2960

2840 – 600

Background in air stored from 4000–2960

Abs. exclude 1500–1350 in Nujol

Exclusions in Nujol: 2960–2840
1500–1350

Acceptable Nujol Scan Regions

OK to Scan 4000–2960
2840–1500
1350–600

Use a 0 to baseline
Scale to CO

June 19 2015

1. The osmosis tube has worked perfectly!
It has risen about 5" ≅ 127 mm
This is quite substantial.

2. Do not forget to copy your file today.

3. What question is does gain affect the background of a scan? Use pityalgene as an example.

Well a gain of 10 gave very nice sharp peaks.
To me it gets rid of lots of the noise.
This is w/ background of 10 gain & scan of 10.
I think that it might be preferred.
Very clean peak presentation!

But the CDB sample is not at all working the same way.

The lesson seems to be do not use higher gain unless you need to. It will distort the reading seen under normal case of samples.

Background of Gain of 10 simply does not work.
It amplifies only CO_2 & H_2O.

Gain of 10 is not working. It is amplifying the background spectra in a [illegible] fashion.

Page 89

In Scale - Offset Menu

y Offset by Factor means subtraction or addition of y
x Scale to Factor means the range from 0 to X

Sample Log

Sample NO	Date	Location
1 ~~FAKE~~	Nov 11 1999	I-5 Central Calif
2	Oct 03 2014	Georgia
3	Apr 25 2014	Australia (Victoria)
4.	Aug 15 2011	Manitoba CA
5.	Oct 16 2009	Sacramento CA
6.	Nov 12 2010	California (a twake)

CDB Protein Recovery Method – Refrigerator

Jul 23 2015

1. Very little protein in small tube (≤1 ml)
2. Fill the small tube to ½ w/ water
3. 4-6 drops 1M NaOH & shake (turns tan)
4. Add 5-6 drops Bradford reagent
   (Reagent turns from red-orange to solution turns blue)

Then verify protein

IR

Sample Processing

We see now that the best way to present the data is

1. Adjust to baseline automatically
2. Scale to approx 0-90
3. Set display limits from 2000 - 600 fingerprint region only.
4. Color each line separately
5. Set tick marks to 100
6. Smooth the data w/ a window of 50.
7. Manually set the peaks.

June 25 2015 Thursday Cabin City MT

Today the interests are:

1. IR spec interpretations - the real McCoy now
2. Osmosis - plan out the experiment
   for both lipids and proteins
3. Ham Radio!
4. Biology experiment
5. Dissection
6. We have books for many interests,
   magazines to catch up with, catalogs
   to understudy
7. Hikes a Cross Country
8. Weather prediction
9. Learn 2 or 3 plants

Highest priority is IR.

Lets go to the COB Signals spectrum

CDB Lipids Jun 25 2015

Sources are:
1. ~~Bell~~ Scan - the big picture
2 - IR Spec
3. Chem Tool 150 x
4. Quick & Easy
5. Coltheup
6. Two detailed textbooks
   Si we have lots of source.
7. IR Pal !!! Good cross correlation

1. We have a very soft linear peak @ 3406
   3300 - 3500 is amide.
IR spec has strongest candidate as an amide.
Si does Coltheup for that matter.
   The amide does look very strong.
2. On ego.
   next is hydrocarbons.
~3100 & 2800 is the major group.

From Key, two sets are indicated here
   2800 - 3000 CH_3 and CH_2

   3000 - 3100 C=C-H this is weak here

One peak are C

3106	~~2871~~	2961	2919	2875 ~~2866~~

Page 94

alkene / vinyl / alkene

positive CH_3
p131 Avram

You have 3 of the 4 peaks assigned now.

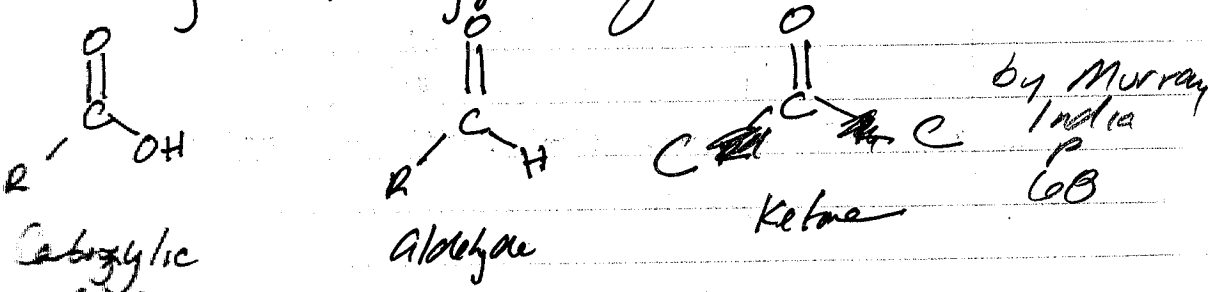
You need 2919.

Most likely CH_2 Koji p 20 @ 2925
yes in this. Ok

Now we have all four peaks.

(3) Next is ~2730.
We apparently have an aldehyde.

An aldehyde is an oxygenated functional



by Murray India p 68

COOH
R-CHO
C9H
RCOR
CO

When we see a ~~test~~ a aldehyde or reduction of a Carboxylic acid when an oxygen is pulled off but a ketone is a reduction of an aldehyde when the hydrogen is pulled off. It would help the properties and Characteristics of aldehyde & ketone are?

This is a good way to remember

Page 95

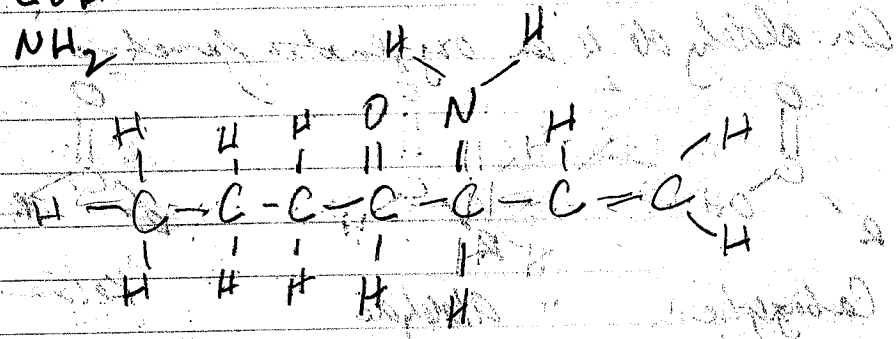
COOH	COH	CO
Carboxylic Acid	Aldehyde (reduction)	Ketone reduction

It is certainly that I have the peaks @ 1720 but not @ 2800 ?
an aldehyde.

But I do have a sharp carbonyl @ 1720.

We are through the group again now.
We have

~~C=H~~, CH_2, CH_3
C=C
C=O H
NH_2



7(12) = 84
14(1)
16(1)
14(1) = 114
= 120

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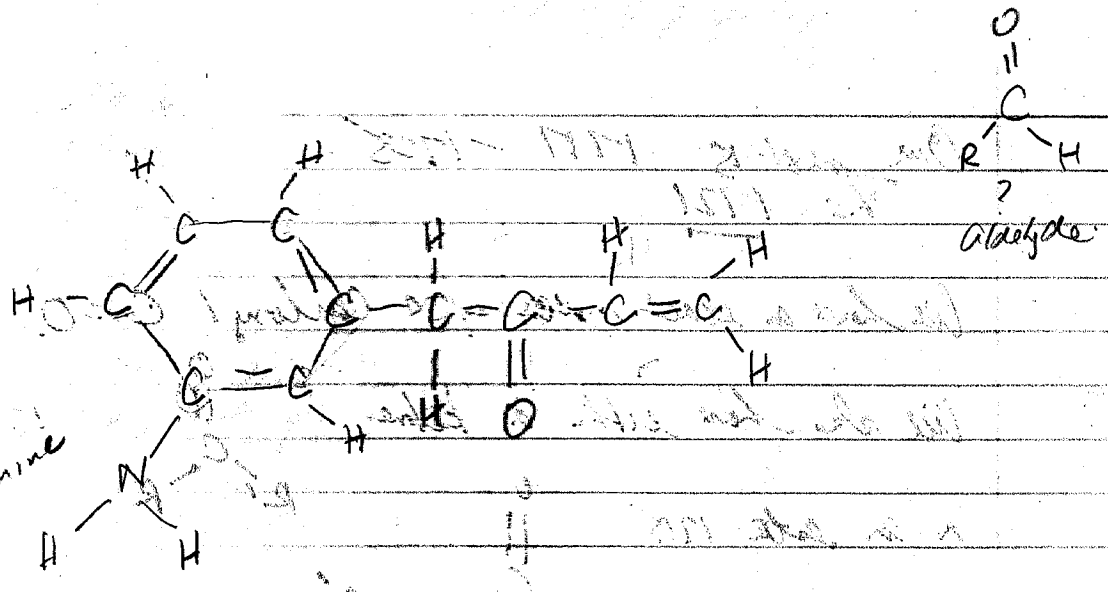
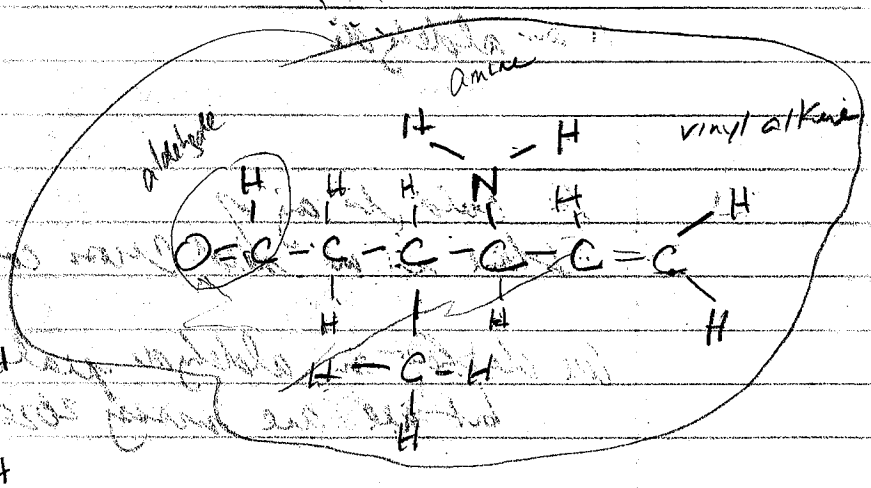
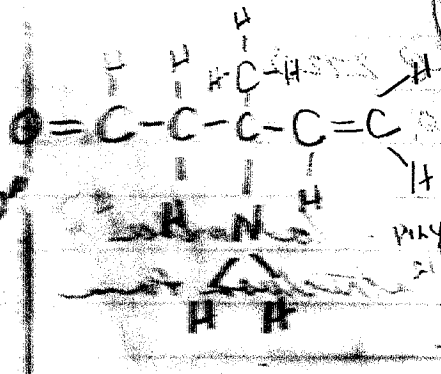


This could be on the right track.

C	9(12)	= 108
H	9(1)	9
O	16(1)	16
N	14(1)	14
		= 147





C	7(12)	= 84
H	10(1)	= 10
N	1(14)	= 14
O	1(16)	= 16
		= 124

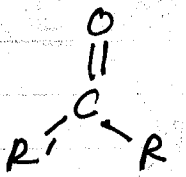
Not bad

This does seem to be a minimalist structure.

Our unk 5 1717 – 1725
X = 1721

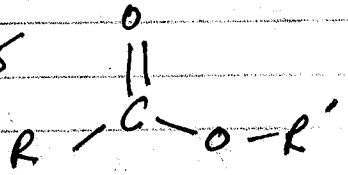
Will have an exact match w/ a Carbonyl C=O.

Will also have either a ketone

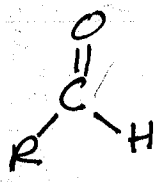


1715-1725

∧ an ester 1715



∧ an aldehyde

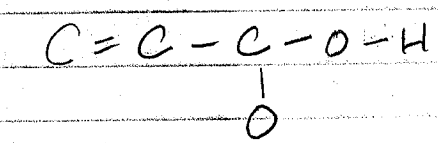


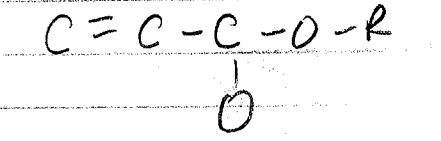
1725-1730

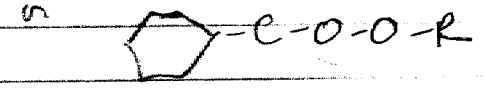
It could be any of these as we don't cross correlation.

We do have an aldehyde peak @ 2720 but we are missing 2820.

Now, IR #8 seem to have an ester match @ aldehyde. But different structures than RCOH are more likely.







"Skip to Here Section"
(Look back ~ 6 pages!)

June 26 2015 Cabin City

Now the big question.
Is a Carbonyl always a C=O
or Can it be C-O?

There is a double bond oxygen
your last pick remains an aldehyde.

So we know that we have O for a ketone.
||
C-C-C

but we have evidence of an
aldehyde.

You therefore are now proposing a terminal aldehyde.

I skipped a page!

NOTICE SKIPPED!

... the aldehydes @ 2720 & 2820 (not found @ 2820)

But now I see that the Partition Chart is for
STRETCHING vibrations only!

Partition
Pavia's Chart on page 17 is far superior.
It shows the big picture of the bands that we
are looking for.

Seems to me this chart should be adjusted to!

Davis Partition Chart

but Stretching Vibrations Only! (it's a start...)

I have modified this chart to incorporate aldehydes.

4000 - ~~2500~~ 2820 — Single bonds:

OH

NH

CH

2820

~~2500~~ - 2000 — Triple & Double Bonds

$C \equiv C$

$C \equiv N$

$X = C = Y$

X & Y can be C, O, N, S

2000 - 1800 — Very Few Bands

1800 - 1650 — Double Bond

$C = O$

1650 - 1550 — Double Bonds

$C = N$

$C = C$

$N = O$ (over-lap below)

1550 - 650 — Single & Double Bonds

$N = O$ (over-lap above)

$C - C$

$C - N$

$C - O$

$C - Cl$

There is an exception found here. Aldehydes are stretching @ 2720 & 2820 and they have a double C=O bond! So be careful; this is only a guide.

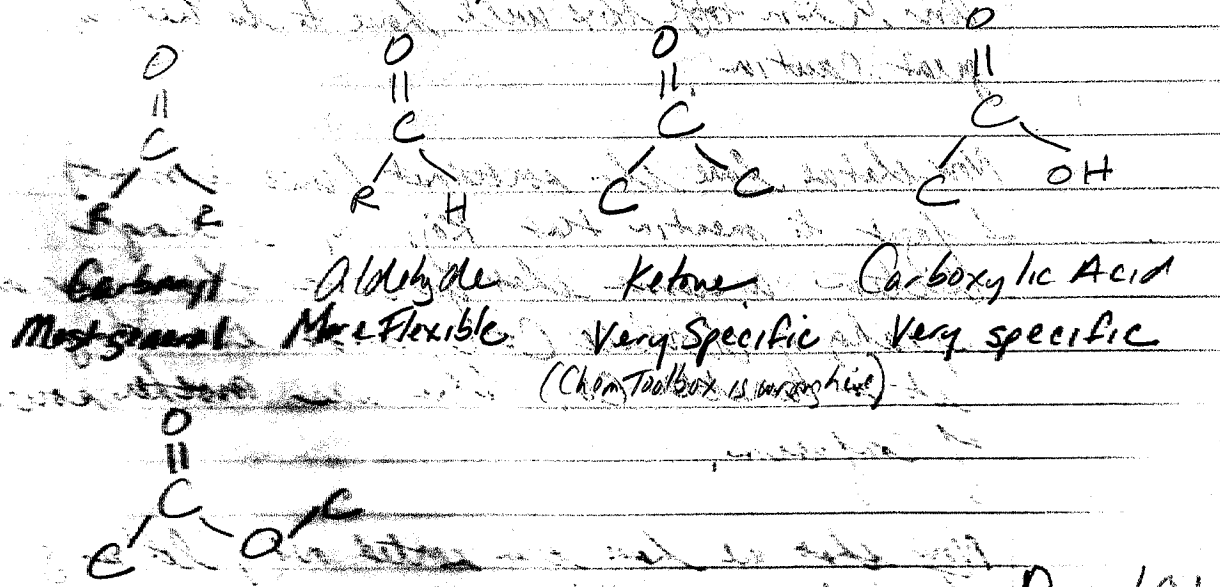
Note: Aldehydes are also @ 2720 & 2820. Aldehydes have a double C=O bond!

Now, the fact that we have a aldehyde indicated @ 2720 (we are running 2020) tells us, from Pavia's chart, that this is not a stretchy vibration. - Because an aldehyde has a double C=O bond & there are no stretching double bond in Pavia's Chart in this region.

So what is it?

By the way, a Carbonyl group is a C=O
We see that definitions are vary & this causes confusion.
Murray wins! Chem Toolbox has some issues here w.r.t. to an "R" group vs a Carbon group.
They appear to not be used accurately.

Murray India wins



A combination of double & single oxygen bonds.

Now we have some of the carbonyl, aldehydes, ketone, ester, double & single bond & partitive chart issues sorted out.
We realize that is confusing. Even Dovia's partition chart seems to have an oversight w/in it related to aldehydes.
Ya also had a problem w/ lower designation of functional groups w/ varying interpretations of "R" groups vs Carbon groups.
What we learn here is that Chem Toolbox appears to have some problems w/ it. It does not seem to be an reliable.

I think we must be Mindful & use reference & designation of functional groups from now on. Chem Toolbox will have to be used w/ great caution.

Now that we have the sorted out (well almost) I forgot to mention that Koji w/ Carbonyl section assume that you know that you are speaking of double C=O bonds even though it is hardly ever CO. This was another source of confusion.

Now that we have this sorted out, let's go back to interpretation.

Page 103

What exactly do we have.

Let's go back to 2720.
IR Pal

The typical value for an aldehyde -CHO (means C=O) is indeed listed as 2720 ± 10. The secondary value is listed at 2820. So we do not pick up the secondary value but that may not be at all unusual.

OK, the 1725 now provides strong confirmation of the aldehyde RCHO @ 2720. I am now confident in the aldehyde.

(5) Let's move on to 1610.
Very interesting. A strong statement of 1611 as a 5-ring alkene.
There is a very interesting twist to the matter.
Notice that it says that it is weak.
But that amine & amide are strong.

We have an interesting situation developing @ 1610.
There is a weak 5 ring situation popping up, but would that not make a lot of sense.
@ 3016 via Jacobs evidence of an alkene.

But our strong peak @ 1610 corresponds with either an amide or an amine. And the amide matches at 3400

Looks @ Quick + Easy,
the case for an alkene is very strong.

The [illegible] fat has many variations here.
Amides are also strong.

The case for alkene is very strong

But what about amines & amides?
I think we should study Pavia & representative samples of
1. alkenes
2. amine
3. amide.

Ok, the amides & amides are not matching up. The NH peaks around 3300 - 3500 are different & strong & these are not showing up.

This is important because this shifts the weight of ~~this~~ 1610 in IR peak towards a 5 ring alkene. This is potentially very significant.

Page/04

June 27 2015 Field Day is now over.

We see now that the fingerprint region of the CDB lipids is quite complex and that is the contradiction.

We are generally quite ok with the alkene, (vinyl alkene remain to be proven), the alkane are fine, the carbonyl w/ the aldehyde are fine; the aldehyde is fine.

What gets very interesting is the 1610. The strongly suggest a 5 ring structure, conjugation is also an issue. 1610 comes from two sources, IR Pal and Avram. The difficulty comes from the fact that Avram has the associated symmetric stretch @ 3061. But notice the asymmetric CH is not listed. And our CH @ 3016. Or maybe the table is that it is an asymmetric CH. This might make sense w/ a terminal alkene attached to a 5 ring structure (likely conjugated).

So let's learn about symmetric vs asymmetric & example of each. Also the focus is on 3016. What exactly is happening here? Sym. or Asym?

June 29 2015 Monday

Continuing w/ the IR work.

Certain patterns are beginning to emerge in clusters.

(1) COOH is non-existent, you see that now.

(2) The 3400 zone or an amine group or ester but you also wonder if there is simply a variation or an alkene as demonstrated in quick & easy page. Amines are usually more sharper and stronger.

The well have to be studied further but the likelihood of amine zone will lower now.

(3) The alkane should be fairly standard fare except for 3406 question

(4) The alkenes are a bit interesting topic.
We have prospects of
1. Conjugated bonds
2. Terminal alkene
3. Stereochemistry of one or more alkene
4. Vinyl alkene

There are many to ponder

(5) Very strong evidence of aromaticity should emerged

6. Other types that have emerged, but not
@ all peaks are
1. Ketones (remember them?)
2. Benzene
3. Nitro Aromatic
4. Alkyl halide

Now, let's continue.
Let's go back to this 3406. 3016

1611 passes the 5 ring alkene rocks strongly
but the 3406 needs to be figured out. 3016
1. Alkene?
2. Vinyl alkene?
3. Asymmetric required per Avram it seems.

Start w/ Koji Again:
Remember we could have both:
vinyl alkene & 5 ring

Last of all, from Avram we have two
choices,
alkene or Arene.
Time will tell.

Now from the AVRAM chart on p 120 we can see
that alkene & arene both have overlap in
the same region. But we can see that alkene extends
into the 900-1000 range but aromatics do not.

We see that we have only one weak absorption in the 900 region.
They are a pair at 895
& 905

What we see in IR pal is that the aromatic is strong @ 3016, and the alkenes are weak.

Ours is strong. This can't be weight toward aromatics.
Our closest match in the aromatic is
from 865 to 875 vs 895 to 905
This is a 1,2,3,4,5 pentasub.

Remember there is an incredibly weak band. 1,2,3 trisub
trans RCH=CHR Aromatics

Stay on the main bands

		theory	meas	theory	meas
		Alkenes		Aromatics	
IR pal	~~trans RCH=CHR~~	3020	3016	✓3000-3100	3016
		1660	1615	✓1600-1585	✓1615
IR pal	~~Aromatic 1,2,3 trisub~~	675-725	700	✓760-780	775. + more

We can see here that the weight is actually somewhat strong toward the aromatic. But neither should be elevated. Maybe you can have both.

There is a Can't Not Can be made for both to exist.

There is no correlating 5 ring structure for trans alkene

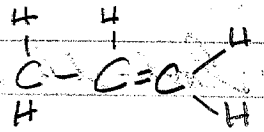
Our current scores are

			Notes
	COOH	30%	
	Amine (1st Group)	82%	Inv. Strength of reading
	2nd Group	81%	" " "
✓	Alkane	90%	
✓	Alkene Group 1 also combined	87%	C=CH
	Group 2	87%	Vinyl alkene
91% now	Group 3	84%	5 Ring alkene
	Group 4	84%	trans RCH
✓	Aldehyde	92%	
	Ketones	61%	
Combined Score is 89%	✓ Aromatics Group 1	57%	These two Groups might combine
	Group 2	66%	
	Nitro Aromatic	62%	
	Alkyl Halide	45%	

Our ranked scores as of now are:

Aldehyde  92%

Alkane CH_2, CH_3 90%

Alkene (Vinyl Alkene)  ~~87%~~ + 91%

Aromatics (Combined)  85%

Nitr. Aromatic 62%

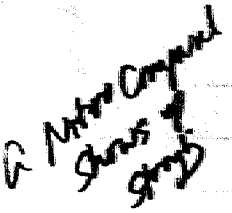
Ketones 61%

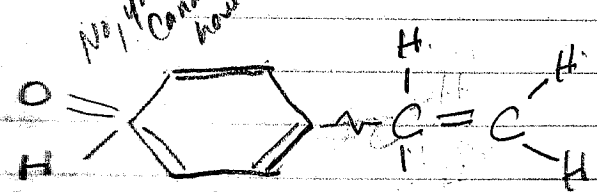
Alkyl Halide 45%

COOH 30%

Amines (Getting weaker now)

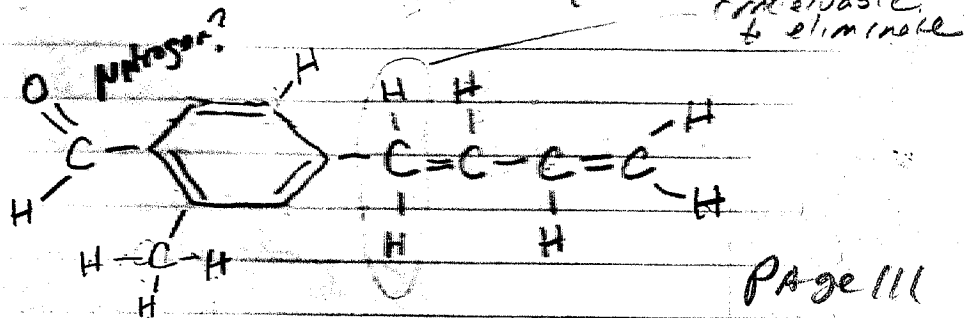
So an initial structural form is 82%





Only Organic Molecule Protein

E(12) = 96
1(16) = 16
1(e) = 0
Σ 120



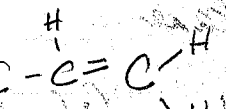
PAGE III

We could have iron added, none C's.

11(12) = 132
1(16) = 16
(10-13)(1) = 10-13
Σ 158 - 161

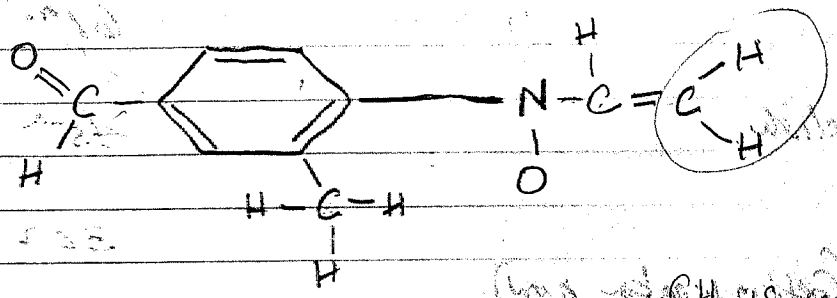
The + stretch to make a lot of sense
Let keep working on the alkene structure

Is vinyl alkene the same as $RCH=CH_2$?
It seems likely.



Yes, it sure looks like it.

Now we have (nitro is conjugated)



CH_2 is in the running + the remaining from 2925 & 1470

10 (12)	=	120
2 (16)		32
1 (14)		14
(9-12) 1		9-12
		175-188

CH_3 is in the running from 2960, 2870, 1

Our best estimate of the molecular weight is

$155\left(\frac{1.80}{1.67}\right) = 167$ error is $\sim 16\left(\frac{1.8}{1.67}\right) = 17$

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So range is 150 to 184

So I am well within range at 175-178 gms/mole

Jun 30 2015 - Tuesday

The COB spectrum is very rich in detail and the should rely a great deal on sorting out and redundancies

Let's look @ 1225-1210 $\bar{X}$ = 1221

Many choices from Koji:

1	1255-1145	CH_3		NO
6	1275-1200	Vinyl ethers, aromatic ethers.	C-O-C	Possible
? 7	1280-1160	aromatic amines	& 1360-1250	Amines/Amides show
8	1300-1050	ketones ethers.		
9	1300-1200	Aromatic N oxides		
12	1240-1190	P-O-C		
12	1300-1180	P=O, POOH		
13	1400-1100	C-F		a bit of a land mine

So then, therefore, in all over the map. taking place here.

from Avram:

$(CH_3)_3CH$

$C_6H_4X_2$

Aryl Halogen $C_6H_3X_3$

C-F

Phenols

Aromatic Ester

SO_3H

R-NO

Aromatic tertiary amine

$R_3N \rightarrow O$

R-CHO aromatic

Ester acetate

In IR Pal, 1221 also causes some problem.

Candidates are

1. Alkyl halide halide R-F

~~2. Amines~~

3. Ethers Ar-O-R 1220-1260

There does appear to be a strong correlation w/ aromatic

~~4. Phosphorus~~

No corollary from 2440-2260

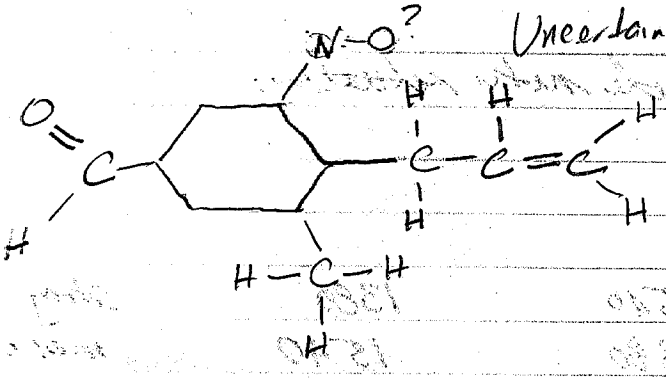
5. N-O aromatic

also strong aromatic relationships

~~6. COOH~~

1. Alkyl Halide CH_2-X

This strongly suggests an aromatic b/c a NO attached to it.



Uncertain Here.

vs aliphatic NO?

Our scores now are.

Aldehyde	92%
Vinyl Alkene	91%
Alkanes	90%
Alkene	87%
Aromatic	85%
Ethynyl Alkene	84%
Nitro Aromatic	62%
Nitro Aliphatic	55%
Ketones	61%
~~Nitro Aliphatic~~	~~55%~~
Ar-O-R Ester	32%
Alkyl Halide	29%

Page 115

Let's look @ the nitro substitution:

Aliph. Nitro	1540	1380	strong
	1380	1540	medium
Aromatic Nitro	1520	1350	medium, strong
	1350	1520	medium, strong

We have
1500 strong
1380 medium

Aromatic Nitro is in range almost on both accounts
Aliphatic is slightly more out of range on the strong stretch

I have 3 peaks. If I combine them together I have

~~(1.5) 1500 + 1~~

$$\frac{1(1500) + .66(1517) + .9(1475)}{1 + .66 + .9} = \underline{1495}$$

for the main peak.

Page 116

My smallest peak is ~ $\frac{1380 + 1370}{2} = \underline{1375}$

TOF Analysis.

IR Pal

Our last two peaks are @ 770 & 700.

@ 700.

Alkenes are strong.

Aromatics are strong

Analyzing the Cross Correlation indicates to me that we should have.

700 vinyl (Alkene)

Then we need 3025-3015 which are here for a further vinyl alkene.

Then we should have another @ 1660.

But we do not. We have appox 1620.

But then when you look @ aromatics @ 700 we should have a 1592.

I believe this will shift the 1660 downwards

1660+ 1592 $\Rightarrow \bar{X} = \underline{1626}$ right where we are.

Theory Alkene Theory Aromatic

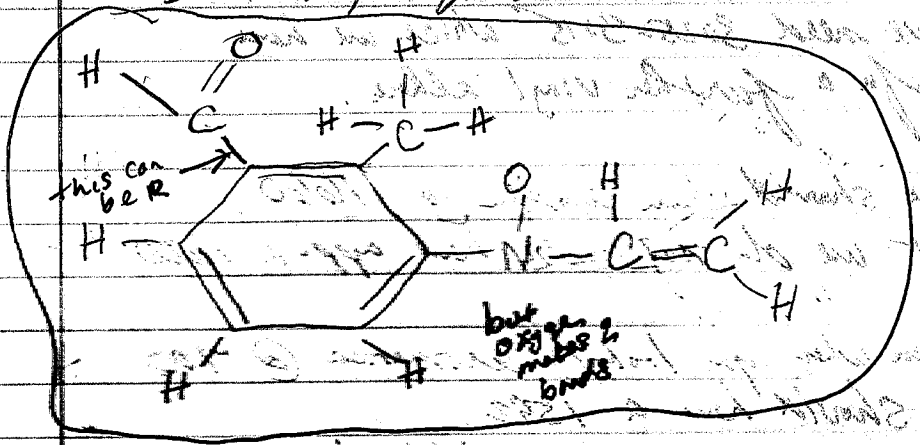
We have a vinyl alkene and an aromatic together.

Nice look @ 770 12 Feb

Group 1,2,3 trisub aromatic shows up.

You also have a meta here
3000 - 3100 Match w/ aromatics
1592 meta w/ our average
770

Si the weight does shift towards



Our best model to date

$10(12) = 120$
$2(16) = 32$
$1(14) = 14$
$10(1) = 10$
$\Sigma\ 176$

$150\left(\frac{1.80}{1.67}\right) = 162$

Theoretical MW = 162

But error is $\left(\frac{1297}{5}\right)^{1/2}$ rms $= 16.1\left(\frac{1.80}{1.67}\right) = 17$

So our 10 range is expected to be 145 to 179.

Most Current Model June 30 2015

$$RMS = \sqrt{\frac{\Sigma x^2}{n}}$$

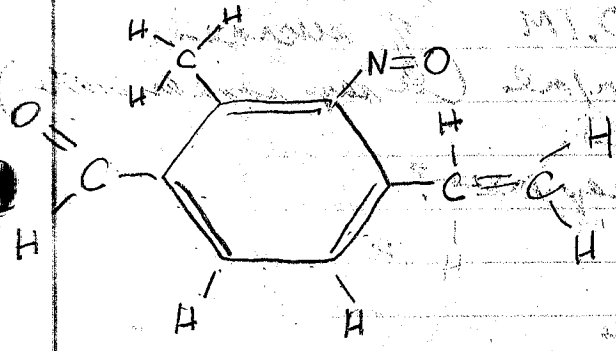
5

5

We are exactly w/in the range of error that we expect to be.

Questions.

1. What exactly is an aromatic NO?
2. How does O maintain two bonds?
3. How do you measure tri substitution
4. Where would an iron attach?



This is our most current structure. It should be on the right track. It would be a 1,2,3,4 substitution.

10 (12) = 120
2 (16) = 32
1 (14) = 14
9 (1) = 9
$\Sigma = 175$

Theoretical MW = $150\left(\frac{1.80}{1.67}\right) = 162$

Expected $\sigma_{(RMS)} = 17$

Range: Page 119
162 − 17 = 145
162 + 17 = 179

Chemistry

Osmotic Pressure. Thinkwell Disc 5 #2910 follow

We are now on to osmotic pressure & the determination of molecular weight. We start w/ Thinkwell.

$\Pi = MRT = d g L$

Thinkwell Example:
Osmosis is the most sensitive colligative property.

Maple tree.
Conc. $= 3^{\circ} = 0.1M$ of sucrose
(marble aqua water) density = 1.03 gm/mL (he says same as water)
Temp = 20°C
How high will the sap rise?

$\Pi = MRT$

$\Pi = \left(0.10 \frac{mol}{liter}\right)\left(.0821 \frac{l \cdot atm}{moles \cdot K^{\circ}}\right)(293^{\circ}K)$ Gas Constant units?

$= 2.40$ atmospheres

$2.40 \text{ atm} \left(1.013E5 \frac{Pa}{atm}\right) = 2.44E5 \text{ Pa} = d g h$

Page 120

Convert to Pascals

$2.4E5 \frac{g}{m s^2} = 1.0 \frac{gm}{cm^3}\left(10^{-3} \frac{kg}{gm}\right)\left(1E6 \frac{cm^3}{m^3}\right)\left(9.8 \frac{m}{s^2}\right) \cdot h$

$h = 24.8$ meters
$= 25$ meters

He forgot convert to kg!

He started off in cm units!

Osmotic Pressure

Dean Harmon made 2 errors!

Now let's repeat the example

$\Pi = MRT = d g h$ (molarity)

We therefore believe our final units of pressure should be $\frac{kg \cdot m}{s^2}$

We have a 0.1 molar solution of sugar

The gas constant is $\frac{8.3145 \text{ Joules}}{K^\circ \cdot mol}$ or $\frac{8.31 \text{ Joules}}{K^\circ \cdot mol}$

g is $9.81 m/s^2$

5.

$\Pi = \frac{0.01 \text{ moles}}{\text{liter}} \cdot \frac{8.31 \text{ Joules}}{K^\circ \cdot mol} \cdot 293^\circ K$

$= \frac{24.35 \text{ Joules}}{\text{liter}} = \frac{kg \cdot m^2}{s^2 \cdot m^3 \text{ per liter}}$

$= \frac{24.35 \text{ kg}}{s^2}$

Question: how many m^3 per liter?

1 liter = 1000 cm^3 = $1000 \cdot (1E{-}2 m)^3 = .001 \frac{m^3}{\text{liter}}$

$= 24.35 \frac{kg \cdot m^2}{s^2} \cdot \frac{(1 \text{ liter})(.001 m^3)}{\text{liter}} = \frac{24.35 kg}{s^2 (.001) m}$

Pressure = $\frac{\text{force}}{\text{area}}$ per unit area.

Force = m · a

What is pressure? $\frac{\text{force}}{\text{area}}$

~~Force · area~~ Force/area

$\frac{kg \cdot m}{sec^2}$ m · acceleration

$\frac{}{}$ area

$\frac{\text{newton}}{m^2} = \frac{kg \cdot m}{s^2}$

$= \frac{kg \cdot m}{s^2} \cdot \frac{1}{m^2} = \frac{kg}{m \cdot s^2}$

This should be pressure units

$\frac{\text{Newton}}{cm^2} = \frac{kg \cdot m}{s^2}$

$cm^2 \cdot 1E4$

$= \frac{kg \cdot m}{s^2 m^2} = \frac{kg}{s^2 \cdot m}$ OK

A Joule is a unit of energy (work)

Energy = force · distance

(Joule) = ~~m~~

$\text{Joules} = \frac{kg \cdot m}{s^2} \cdot m$

$= \frac{kg \cdot m^2}{s^2}$

Page 121

$= \frac{24350}{m s^2} kg$

This is a unit of pressure

In fact an answer of

$\frac{2439\ kg}{m \cdot s^2}$ which by value we have figured out is indeed a unit of pleasure.

Now we have $\frac{2.4E5\ gms}{m \cdot s^2}$ which for us would be $\frac{24350.0009ms}{m \cdot s^2}$

which would be $\frac{2.435E1}{m \cdot s^2}$ which is not the same

so we have a problem. Why? a factor of 100.

$1\ m^3$ to cm $= (1E2)^3 = 1E6\ cm^3 = 1000$ liters

The problem is the gas constant.

We use .0821 $\frac{l \cdot atm}{mole \cdot K^\circ}$ I use 8.31 $\frac{Joules}{K^\circ \cdot mole}$

Our constant is large by a factor of 100. let's figure out why or, we found his value in our science text book.

Somehow: $\frac{8.31\ J}{K^\circ \cdot mol} \stackrel{?}{=} \frac{.0821\ liters \cdot atm}{K^\circ \cdot mol}$ Why?

$\frac{kg \cdot m^2}{s^2 \cdot K^\circ \cdot mol} \stackrel{?}{=}$

This means that somehow

$$\text{liters} \cdot \text{atm} \cdot .01 \overset{?}{=} \text{joules}$$

1 cu. meter = 1000 liters (OK, we knew that right)
1 liter = .001 m^3 (OK so that also)

So

$$.001\ m^3 \cdot \frac{10332.3\ kg}{m^2} \cdot .01 = .1033\ m \cdot kg \left(* \frac{m}{s^2}\right)$$

(* acceleration due to gravity)

↑ this term is needed to make them equatable

Force = $\frac{kg \cdot m^2}{s^2}$

What we are learning here is that the Gas Constant actually is defined in different forms of units. I think that Dolores in our Chemistry class warned of use of this.

It truly can have two different values and the only way we had a difference of ~100. (101.325?)

R of $\frac{8.3145\ \text{Joules}}{K^\circ \cdot mol}$

IS NOT THE SAME AS

R of $8.2057E{-}2\ \frac{\text{Liters} \cdot \text{atm}}{K^\circ \cdot mol}$

So my answer was actually correct, in terms of the gas constant that I used!

But to use in Constant, it would have had to take my answer of

$$= \frac{24350\ kg}{m\ s^2}$$ but we needed to divide it by a factor of 101.3259

So we would then get

$$\frac{240.3\ kg}{m\ s^2} = \frac{240314\ gms}{m\ s^2}$$

$$= \frac{2.4E5}{m\ s^2}$$ and the scaled is the answer!

Then we really stuck.

Page 24

Now that we know that R is a very tricky gas to handle, we can move on.

Now he went on to equate to pressure of height.

$$2.4ES\,\frac{gm}{m\,s^2} = d\,g\,h$$

d: $\frac{gm}{cm^3}$, g: $\frac{m}{s^2}$, h: meters

If we change cm to meters we should be ok... & gm to kg

$$2.4ES\,\frac{gm}{m\cdot s^2}\left(\frac{1E\text{-}3\,kg}{gm}\right) = \frac{gm\cdot\left(1E\text{-}3\,\frac{kg}{1\,cm\,gm}\right)}{\left(cm\cdot 1E\text{-}2\,\frac{m}{cm}\right)^3}\left(\frac{m}{s^2}\right)(m)$$

$\frac{kg\cdot m^2}{m^3\cdot s^2} = \frac{kg}{m\cdot s^2}$ OK

$\frac{kg}{m\,s^2} = \frac{kg\cdot m^2}{m^3\cdot s^2} = \frac{kg}{m\cdot s^2}$ yes, this works.

$$h = 2.4ES\,\frac{gm}{m\,s^2}\left(1E\text{-}3\right)\frac{kg}{gm}\,\frac{m^3}{kg}\left(1E\text{-}6\right)\left(\frac{1.00}{1E\text{-}3}\right)\frac{s^2}{9.8\,m}$$

OK!

.025 and he has 24.8 meters

∴ I am off by a factor of 1000.

Look figure out factor of 1000. Why?

$$245\,\frac{kg}{m\cdot s^2} = d\,g\,h \qquad d = \frac{1gm}{cm^3} = \frac{1E\text{-}3\,\frac{kg}{cm^3}}{(1E\text{-}2m)^3} = 1000\,\frac{kg}{m^3}$$

$$1000\,\frac{kg}{m^3}\cdot\frac{9.8m}{s^2}\cdot h$$

Page 125

$h = .025$ meters – what is wrong here?

$\frac{2.4E5\,g}{m\,s^2} = 1.0\,gm$

Hold on here.
I believe Dean Harmon is wrong on two accounts. His units are wrong

I believe twice!
Lets start over.

I believe that our first answer was correct. If we have an answer of

$\frac{24350\,kg}{m\,s^2}$ I actually believe that Dean is wrong by a factor of 400.

Now I believe that we continue we now have

$\frac{24350\,kg}{m \cdot s^2} = d \cdot g \cdot h$

$h = \frac{24350\,kg}{\frac{m \cdot s^2}{\left(\frac{1000\,kg}{m^3}\right)\left(9.8\,\frac{m}{s^2}\right)}} = 2.49$ meters

And Dean is wrong. He got 25 meters and he is off by a factor of 10.

The only way that the maple tree will get the syrup is if it is a 1.0 M solution, not a 0.1 M solution!

This make perfect sense. A 0.1 M sugar solution would never rise 75 feet up in the air. But a 1.0 M solution would.

What is the molar mass of sucrose?

Jun 30 2015

Environmental Samples - First Pass.

· 3272 Polymeric OH T5(3)

strong, broad	Alcohols & Carboxylates	3200 - 3650
weak & medium	Amines	3000 - 4000

Thurs JU 01 2015
Environmental Filament - First Pass

3272 Polyvinyl Alcohol Koji, Avram

2923 CH_2 Koji

1648 Alkene
terminal vinyl alkene D24 Koji
terminal methylene D24 Koji

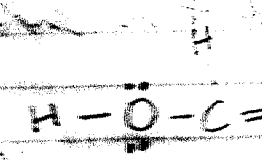
1520 Aromatic Nitro IR Spec

1230 C-O Aromatic IR Spec

1167 C-O Alcohol IR Spec

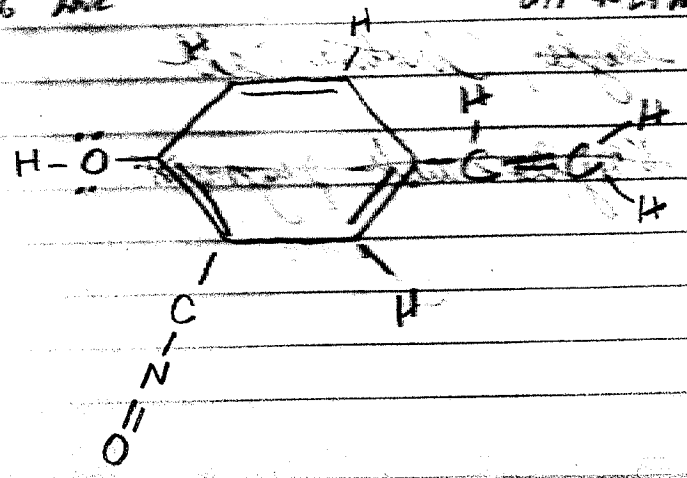
1011 C-O alcohol IR Spec

From Chemistry, Brown p357, Vinyl alcohol



Seems like this is a first pass that combines all features

What I'd want to have



Environmental Filament Prospect

July 01 2005 Back in Wallace

What is on our plate?

Meds
Glasses
~~Hard Drive~~
~~Milk~~
Stylus
Beakers?

1. Browse the [illegible] catalog
2. Check the [illegible] order status
3. ~~Check the [illegible] order status~~

4. The [illegible] prospect.
Maybe test them w/ another set of solvents.

This is going to be a very important experiment.
You may be able to do it with no proteins [illegible].
Test it with milk

Vit C
5. ~~[illegible]~~ [illegible] in the teeth. ~~[illegible]~~?

6. ~~Dr. Martin call.~~

7. ~~Dr. Walker call, [illegible]~~

8. Lipid analysis [illegible] research to no end.
"White paper"

9. The environmental filament project [illegible].

10. ~~Kaylee~~, Christine Call

11. ~~Kaylee - web payment~~

July 01 2005 Back in Wallace

What is on our plate?

1. Browse the key catalog
2. Check the key order status
~~3. Check the tent order status~~

4. The ocmoses prospect.
Maybe test idea w/ another set of solvents.

This is going to be a very important experiment.
You may be able to do it with no proteins soln.
Test it with milk.

Vit C
5. ~~Clove acid in the teeth~~. ~~Tea Tree Oil~~?

[redacted]

8. Lipid analysis a research to no end.
"White paper"

9. The environmental filament project ligense

[redacted]

Need
Glasses
~~Heat Dome~~
~~Milk~~
Stylus
Beakers?

12. Edvotek salvo - [redacted]

[redacted]

1. Research paper
2. All comparisons possible w/ found paper
3. IR/filament analysis

1. Protein Diversity
2. Molecular ~~determination~~ of proteins - Sound good?
3. Another one we have!
4. Cleavage of DNA
5. Electrophoresis.

13. ~~Pick up Helium - GC setup~~?

14. ~~Look @ catheter~~

15. Best data to collect on IR?

16 ~~Does a rubber band dissolve in acetone~~
~~a ~~xylene~~?~~ Membrane drier out

[redacted]

Osmosis experiment.

I have now set up the osmosis experiment.
I have made a solution of powdered milk.

1.05 gms powdered milk
100 ml of water.

View properties of your COB model.

Why the change in molecular weight

Current @ 5.5 mm height 29°C

Pressure $\frac{kg}{m\,s^2}$

$\Pi = MRT = \rho g h$ $M =$

Work backwards

$M = \frac{\rho g h}{RT} = \frac{1.0\,gm}{cm^3}\,\frac{(1E-3\,kg)}{gm}\,\frac{1\,kg}{m^3}$

$= \frac{1.0\,gm}{cm^3} \cdot \frac{1E-3\,(kg/gm)}{(1E-2)^3\,m^3/cm} = \frac{1000\,kg}{m^3}$

$= \frac{1000\,kg}{m^3} \cdot \frac{9.8\,m}{s^2} \cdot .005\,m$

$\frac{8.31\,\frac{kg \cdot m^2}{s^2}\;302^\circ K}{K^\circ \cdot mol}$

$\frac{gms}{liter} = \frac{kg}{x\ m^3}$ same

In Chemspider I found a reasonable partial match to CDB lipids.

It is called 3 Nitro 2 Vinylbenzoic acid

Method:

1. Advanced Search
2. Load file
3. Set to Similarity
4. Set Similarity to 80%. Search by Tversky
5. Hit Search @ bottom

$$= \frac{1000\ kg}{m^3} \cdot \frac{9.8\ m}{s^2} (.005m) \cdot \frac{K^\circ \cdot mol}{1} \cdot \frac{1}{8.31 \frac{kg \cdot m^2}{s^2} \cdot 302^\circ K} \quad \frac{kg}{m^3}$$

$$= \frac{1000\ kg}{m^3} \cdot \frac{9.8 m}{s^2} (.005m) \cdot \frac{K^\circ \cdot mol}{1} \cdot \frac{s^2}{8.31 kg \cdot m^2 \cdot 302^\circ K}$$

$= 3.905$

But we know M. It is $\frac{10.5\ gms}{1000 ml}$ so it is a 10.5 m solution

We got 3.905
This says that it will rise to 13.45 m before it is all done.

$1\,m^3 = 1000$ liters

m is molality = moles / per kilogram

$1\,m^3 = (10^2)^3\,cm^2 = 1E6\,cm^3$ $\quad 1E6\,cm^3 = 1000$ liters

Units help only when units get right

$\Pi = MRT = dgh$ $\quad M$ is molarity = moles per liter

we know h, g, d $\quad d = 1.0\,gms/cm^3 = 1E6\,gms/1E6\,cm^3 = 1000\,kg/m^3$

this means we know Π

$M = \frac{\Pi}{RT}$ $\quad$ as we learn $M = \frac{gms}{liter}$

$h = 6.6m$

$\Pi = \frac{1000kg}{m^3} \cdot \frac{9.8m}{s^2} \cdot (.0066m) = \frac{64.68\,kg}{m \cdot s^2}$

This is the current osmotic pressure.

Now

$$M = \frac{\Pi}{RT} = \frac{\frac{64.68\,kg}{m \cdot s^2}}{\frac{8.31\,kg \cdot m^2}{K \cdot mol \cdot s^2} \cdot T^{\circ K}}$$

$$M = \frac{64.68\,kg \cdot s^2 \cdot K \cdot mol}{m \cdot s^2 \cdot 8.31\,kg \cdot m^2 \cdot (T = 302^\circ K)}$$

$$M = \frac{mol^*}{m^3} = .025773\,\frac{mol}{m^3} = .001\,\frac{}{liter}$$

So we need to divide our value by 1000 to get moles per liter

$$M = \frac{moles}{liter} = .000026\,\frac{moles}{liter}$$

powdered milk

so $\frac{1.05 \text{ gms}}{\text{solvent } 100 \text{ ml}} = \frac{10.5 \text{ gms}}{1000 \text{ ml}}$ is to current solution.

but this represent a .000026 M. Solution

Si a 1M Solution is

$\frac{10.5}{.000026} = \frac{403,846 \text{ gms}}{\text{liter}}$ is our estimated Molecular Mass Certainly a huge number.

Bottle process has worked!

The composition of low fat Milk powder is

50% lactose 342 gm/mol
35% protein 82% casein, 18% whey
8.5% Ash
3.5% Water
3% Fat

14,000 to 120,000 is a lot more common

Mycoplasma is 46,000 gm/mol

(casein can range 23,000
lactalbumin is 90,000
Some of the constituents is to 100,000 to 1 million
but most are not

They are on value seem a bit high

$\frac{10.5 \text{ gms/liter}}{.000026 \text{ Mole-Solution}} = \frac{X}{1 \text{ Mole-Solution}}$

Page 135

$X = 404,000$ Very high but not impossible

If the column rises higher, the molecular mass will be smaller

I would estimate that the column should rise by a factor of 10 ≅ 5cm.

It seems to me that this method is very effective & probably a lot easier than electrophoresis.

But it's always good to know more than one way of doing things.

Would you like to try another method?

Latest measurement is 8mm.
This change it to 336,109 sms/mole

9.6 now ⇒ 94.08
2517.93

,0314 ⇒ 283103

I could estimate that the column should need by a factor of 10 ≅ 5cm.

It seems to me that this method is very effective & probably a lot easier than electrophoresis.

But it's always good to know more than one way of doing things.

Would you like to try another method?

Latest measurement is 8mm.
This change it to 336,109 sms/mole

9.6 now ⇒ 94.08
2517.93

.0314 ⇒ 283103

Lipid - Osmosis - Molecular Weight Determination.

Start Column @ 1130 on 070315.

Ethanol (denatured) is the solvent

The solute is 10 ml of lipids added to 50 ml of ethanol.

The density of ethanol is 0.79 gms/ml

Lets determine the density of the lipids.

Density of Lipids = 0.85 gms/liter

$C_{10}H_9NO_2$

July 04 2015 Saturday

The [illegible] experiment did not work in the slightest. I have no idea why. How could it make no change whatsoever?

One thing we could do is use ethanol for [illegible] [illegible] then acetone?
Back to the drawing board on this one.

Today:

1. Broken [illegible]? IR

2. Dr.- A GC?

3. Inhibition tests are coming

4. Pricing of equipment is coming

5. Almond IR

[illegible] at ATR worked w/ gain 10..!

Page 138

JUL 05 2005

1. The osmosis molecular experiment did not work. It appears as though the membrane was dried out by the alcohol. I have no alternative to show right now.

2. The ATR of the protein was a complete success. Magnificent work - you see how Sam's effect the result like a letter (or more) as possible to pick up a signal.

False

3. Today we want to try ATR on the GDA filament.

4. After this what would we like to accomplish?
   1. Echotek?
   2. Almond extract idea?
   3. Search on compound & prevent properties & study them?

5. Up on the right track.
   Coming up will be
   1. More induction tests
   2. Purchasing of lab equipment.

Page 139

The ATR is presenting some real challenges. We have no idea what we are getting now.

July 06 2015

[redacted]

2. Urine spectra

3. Blood spectra

4. Edvotek

5. GC, can ya get it working?

It appears though heat of 200°F affected the urine sample. It absorbed way too much IR across the entire spectrum now. There is a possibility that you have been using too much sample. Even blood a great deal, small, looks more than adequate.

JUl 07 2015

1. Saliva & Blood & EPA Glonet.

Done — Repeat on that needed and reduce the sample size for those that did not work.

Done — [redacted] blood & saliva.

3. Do you want to stay to GC today?

4. Edvotek – is it time?
(Clay overdue)

We have both blood & saliva spectra as well as microscopic image of the blood now for Carl & Clifford. That is good work.

Done — We are now going to work on the background scene.

Done — Double KCl Crystals in the holder now.

Conclusion: The gray outside of the KCl is significantly less than that of the background without the KCl.
This will have caused some distortion but it is not severe.

Done Now let's go back to the EPA & reduce the sample size.

Next, what about the time you can use cellophane?

* I have succeeded w/ ATP and Ethanol!!

* Also with the protein powder.

I have modified the backing plate of rubber bands for a seating surface.

July 08 2015

1 Consider the ATR background development with the base plate in mind.

2 Tools we want EPA in ATR

3 Hair in ATR

Now background of ATR base plate with rubber bands but no pressure on plate.

It look identical to the normal air background specimen.

Now we take the ATR w/ pressure on the backy plate and the rubber bands.

There is a difference, but only in magnitude. The ATR Wants pressure has a lower magnitude if $\bar{X} = 10$ instead of ~ 20 for the single beam magnitude.

Page 144

The is all internal.
Now let's put on polystyrene (Dollar Store)

ATR backgrounds are taken w/ a gain of 1

ATR Background No Pressure

Dilla Story polystyrene test ATR

Use NO
Gain 1 Background w/ Pressure on Backg Plate
The signal here is weak and it only picked up the major CH peaks @ 2900.

Gain = 10 Use Background w/ No Pressure
It is better. It picks 5 peaks instead of 2. Not great, but better

Gain = 100 Use Background w/ No Pressure
Then is highly distorted and does not work.

Background
Gain = 1 Pressure on Backg Plate
Quite a bit of noise in the signal.
Not a good spectrum.
Baseline noise

Gain = 10 Pressure on Background Backg Plate

Then is definitely our best spectrum.
Even the water & CO2 are effectively
Cancelled out. This is quite good.

Page 145

We have a lot of a problem of the protein powder & it did not react the same way as the polystyrene
We only have 3 real peaks.

yes, have one w/ 1 scan average.

- 2007 R-N=C=S
- 1879 Nothing
- 868 Aromatics & Amines
- 604 possible Alkynes, Alkyl Halides

Baseline looks good but everything else not as good.
We are out of powder.
Maybe we needed a little more in the sample?

So we have a good spectrum w/ one average. But there is definitely not one of them.

Ther means that the sample amount & placement is a big factor
I do not believe that we had nearly enough sample that time.

July 09 2015 Found the problem.

Ok, you have figured out your known spectrum problem.

You are getting the inverse of the background spectrum.

$O - B = -B$

B stands for background.
It means that your input signal is zero.
Or at the very least,
that your background signal is very large
compared to your signal.
It's effectively no signal.

w/ gain of 10 w/ a low signal

$O - 10B = -10B$

It could be that it is multiplying the background by 10
and that you have a low input signal.
The gain knob need to be multiplied by 10.

What you learned today is that the background spectrum needs to be weakened if you trying to ~~detect~~ detect a very weak signal.

IEZ (Range of ~5) is best on background if primary signal is weak.

Page 147

ATR & Direct are two sides of the same coin.
Explore the range

With ATR I believe that you want the background selected so that the average strength of the signal is on the order of 50 to 100.

Note

There does not appear to be any advantage in having a height I can set.

Yes, then picked up a couple more peaks that we lost otherwise. Very good order.

Combine ATR & Cells as the last word

Note

along with proper selection of background to not swamp the signal

Page 148

$KMnO_4$ is a powerful oxidizer.

158.03 gms / mole so a 1M Solution is 158.03 / 1000 ml

We have 30 grams.
I do not want to use more than 3 gms.

$\frac{158.03}{1000ml} = \frac{3gms}{X}$ $X = 18.98$ gms.

I need approx a 0.1 M Solution.

a 0.1 M Solution is $\frac{15.80gms}{1000ml} = \frac{X}{30ml}$ $X = 0.47$ gms

We could go for a 0.5M solution.

0.5M Solution $= \frac{79.015gms}{1000ml} = \frac{X}{30ml}$ $X = 2.37$ gms

This is fine. Let us make up a 0.5M Solution of $KMnO_4$

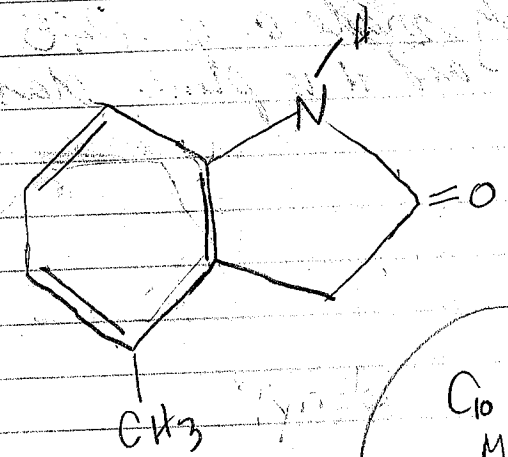
I have already made a 0.048 M solution in water and it is plenty dark.

Jul 12 2015

1. Let's go to SDBS on Lipids

Lmq	I			
		Let's hit major peaks found ~<60		
52	43	3016	3021	15,65
56	46	2961	64	15,60
58	42	2919	62	15,55
32	58	2870	2864	12,55 O
				140 < MW < 200
				12,60 34,45
32	58	1717	1716	p-Acetylbenzoic acid 22991
			174	4-phenylCyclohexane 15612
			183	1,3 Dimethyl-1,3,7 triazaspiro nonane dione hydrobromide 30109
				$C_8H_{13}N_3O_2$
51	49	1495	1490	
(64)	36	760	757	

This was created



This was a match in Chemspider

Page 150

$C_{10}H_{11}NO$
MW 161.2

Now add w/ 12,60 140 < MW 200

1610

691

12,60 140 - 200 No Hits
12,65 ∅ Hits
12,70 4 Hits

18457
7099 benzene, 5 ring
~~15612~~ overlap
~~28~~ 29897

You now have 6 candidates that you can start to look @.
of the 6 candidates 5 of 6 of them have a benzene ring
5 of 6 have nitrogen
4 of 6 have C=O bond
6 of 6 have a methyl group
4 of 6 have nitrogen a/in a ring structure
2 of 6 have a 5-ring structure in addition to a benzene ring.
3 of 6 have an NH

from this →

I believe 1 of them had two benzene rings

1. SDBS
gives you 6 candidates
2. Create generic structure
3. Locate in Pub Chem?
4. Lipid database

Pub Chem database is name only

Quinolinone This must have come from SDBS
quinolin

5 methyl - 3,4 dihydroquinolin 2 (1H) one
This was the meta in Chemspider

Lepadin D pubchem.ncbi.nlm.nih.gov

Pub Chem ID is 42608374
Lepadin D

This must have come from Lipids database

Class: Sphingolipids

1. Med papers

2. Survey

3. Two Links
1. damage to the cell wall n membrane
2. Aerobic respiration
3. Creation of proteins & enzymes
4. Preservation of genetic integrity

Jul 14 2015

[redacted]

X112

2. Programming (at least setting) a repeater w/in Baofeng
3. APRS - we are making progress
4. Sending email by Winlink?
5. Dissection
6. Biology Lab - enzymes
7. Spectroscopy Interpretation
8. Adv. Class Ham license study
9. Send email by APRS to (W6UK-1?
10. Casio
11. Soil Analysis (1/16.91)
12. Music

(1/15.03 packet)

[redacted]

13. Cross country skiing
16. Ham Radio
17. Where is the inverter?

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Jul 16 2015 Bass Creek 2 weeks

1. Soil ~~Tests~~ are underway.
2. Enzyme tests are underway.

---

1. Soil Tests:
The first soil ~~test~~ has been completed. Forest soil Sample.
pH - estimated measurement is ~5.8

Leaves & Grasses Nitrogen (N) - result was nil to low (grass, leafy)

Not Stated Potassium (K) - result was ~~Low~~ nil (roots and stems)

Roots & Stems Phosphorus (P) result was ~~not~~ low

The result from ~~the test~~ was that the forest soil sample was very low in nutrients and that it is on the acidic side.

Low nitrogen means not a leafy & grassy area, which is quite true.

Phosphorus
Some ~~Potassium~~, but still low, is in correspondence with a rock & stone area characteristic of trees & shrubs. The grasses here are very poor.

Potassium purpose is not stated.
The test result was nil.

Conclusion is that the soil in the forest environment is generally poor, acidic & of low nutrients.

It would be beneficial to run some tests in more favorable areas to see if there is any difference - there should be.

You also have a qualitative study of soil taxonomy. You will now be off for many different mineral types.

You have completed the moisture test; it has come out @ ~ 17% moisture.

Note acetic acid use in the next set of preparations

You have an NaOH organic compost in test; this comes out very high w/ a very dark color.

Now we go on to minerals & ions.

1. The nitrate and nitrite tests give a completely negative result. You have test strips for this. Your soil test also gave a negative result for nitrogen. Your water test kit also has nitrates & it is giardia free.

Soil & Enzyme Labs

SOIL: Discovery Topics

You actually have many interesting topics that have been uncovered during the analyses.

soil nutrients.
the lack of them, how they determine the vegetation

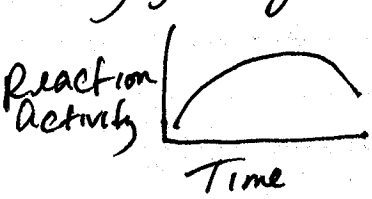
How the forest environment likely differs radically from a gardening environment.

whether reagents are still effective over time.
We had conflicts w/ ppt measurements & potassium measurements using two different test kits.

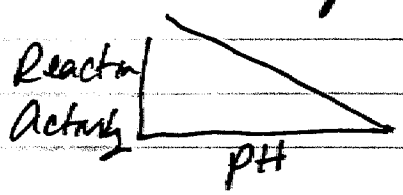
How acetic acid (and I can use vinegar if I need to, & distill @ that if needed) the numerous ions & minerals that were tested w/ the soil kit (Chemical Composition of the Soil) was great.
The tie in w/ aquarium testing & water testing was great.

ENZYME:

1. What an enzyme does (break stays down or facilitate a reaction)
2. How it actually does it by joining with and affecting bond structures, not just some "complete mystery."
3. About lactase tablets, and how we might start looking for them in the store.
4. About sugars: monosaccharides, disaccharides "milk sugar" and how they are broken down into monosaccharides by enzymes.
5. Different ways of measuring glucose & how to start looking for a meter at the store. (We might monitor bacterial culture also).
6. Enzymes are very much dependent upon time, temperature, pH & they are also SPECIFIC.
7. Very good regressions achieved upon



Quadratic worked very well



Linear worked very well.

Jul 17 2015 Friday Bass Creek

Today I saw proven photosynthesis
up Biology Lab #6. by two different
methods.

1. The first is by the visible production
of O_2 by placing the leaf (water based
plant is easier) in a weak solution
of baking soda & then placing this in
the sunlight. This is a marvelous
thing to see and it makes a direct visual
impression and understanding of what
photosynthesis is about.

2. The second method uses the creation of
a vacuum in the leaf that is
subsequently filled up by O_2 (take leaf
piece/disks in a baking soda
solution). The production of O_2 will
cause the evacuated (and therefore sunken)
disks to float to the surface.

This is also a proven photosynthesis and
is a relative measure of net photosynthesis
(Respiration consumes energy).

Page
158

Sphingolipid retracement.

1. SOBS search on myo peaks.

2. 6 Candidates located

3. Selected Common functional groups

4. Created generic structure
held within Avogadro & ACD
Filename ACD-CDB09.SKZ
Smiles file is available from this.

5. Now what happened next is that you found an exact match for the in pub med. USING ACD-CBD09 the number is 10102124 and it is called

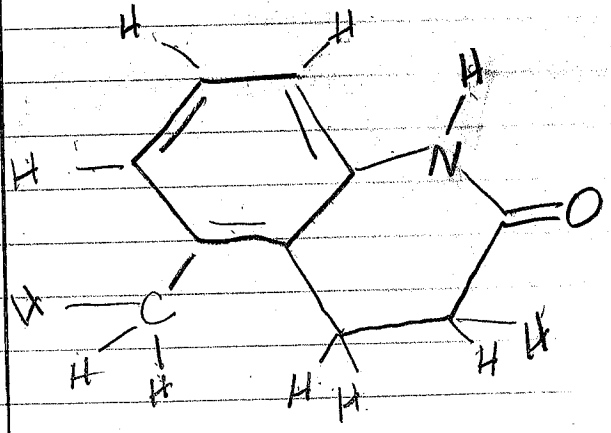
2(1H)-Quinolinone, 3,4-dihydro-5-methyl

It has a MW of 161.2
and formula $C_{10}H_{11}NO$

Noticed the diff in this number vs 42103314

Did you change the structure in any way?

Use the IUPAC name in next page (2)



This is what you want into pub med with.

Page 160

Jul 22 2015

Lipid Retracement

6. The next question that arose is how you connected Pub Med to the Lipid database but you did.
You might have 1. uploaded a structure
2. used a name

Connection to Lepadin must be made.
This took

$C_{10}H_{11}NO$	to	$C_{10}H_{35}NO_2$
161.2		297.5
10702124		42608374
Quinolinone		Lepadin D
Pub Med		PubMed

somehow using the Lipid database in between.

Yes. The link is that the name.
methyldecahydroquinolin IS IN the
Lipid database
as Lepadin D.

Then then went back into Pub Med where
42608374 came up.

Lipid database came up with LMSP01D80052
and the name above.

Page 161

Then we went to Pub Chem & found
with Common name Lepadin D to 42608374
Candidate.
Notice: No Aromatic Rings!

Back to our spreadsheet.

Ok, the rules to match came up.
By text search the Lipid data base
for quinolin, not quinoline

A single match. Lepadin D

Quinoline came up empty in the Lipid
database so I am not sure how
you found this.

Guess what:

The IUPAC name IS (from Pub Med itself)

Use xpcs

5 methyl 3, 4 dihydro 1H quindin-2-one

This is how you found it in
the Lipid database

There are 2 exact matches in pubmed.

It has 8 different names by vendors

Now you know how you found it
in the Lipid database.

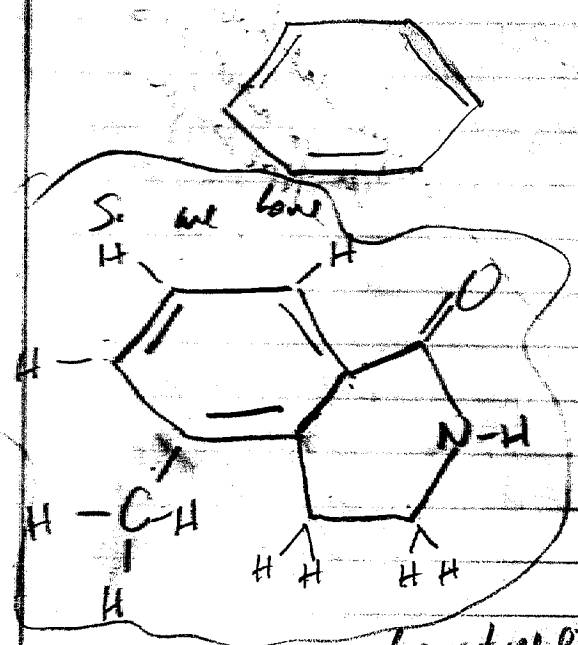
Our question now is to develop an IR spectra interpretation that is CONSISTENT w/ the SOBS approach. It does not have to be an exact match. It only needs to be consistent.

ie

5 of 6 have a benzene ring	83%
5 of 6 have nitrogen	83%
4 of 6 have a C=O bond	67%
6 of 6 have a methyl group	100%
4 of 6 have Nitrogen with a ring structure	67%
2 of 6 have a 5 ring structure in addition to a benzene ring	33%
3 of 6 have an NH	50%
4 of 6 have multiple ring structures	66%

And we have an estimated molecular weight of 162.

We would then go draw:



This is indeed one type of structure.

But since we have a MW estimate of 162

6(12) = 72

We want 6 rings

We surmise it has a ring structure, but not necessarily aromatic

Could be 5 ring also

Page 163

Aromatic MWs 10(12) = 120

1(16) = 16

1(14) = 14

4(1) = 4 = 154

+7(1) = 161

We have confirmed our structure proposal by

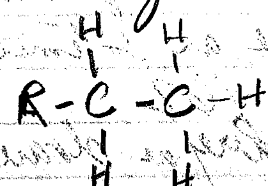
1. SDBS
2. Statistical probability
3. Molecular weight observation.
4. Then led to pub chem notes,
5. Then led to lipid match (regular).
6. Now we go to IR functional group analysis and see [illegible]

Thus far we have candidate of

alkane 79%

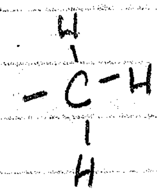
We have

RCH_2CH_3



and

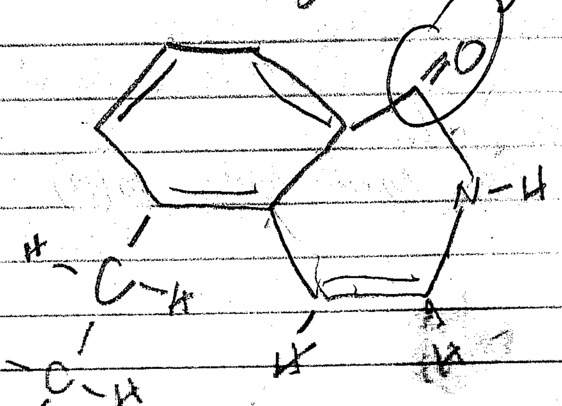
CH_3



as candidate

This would change our structure to be:

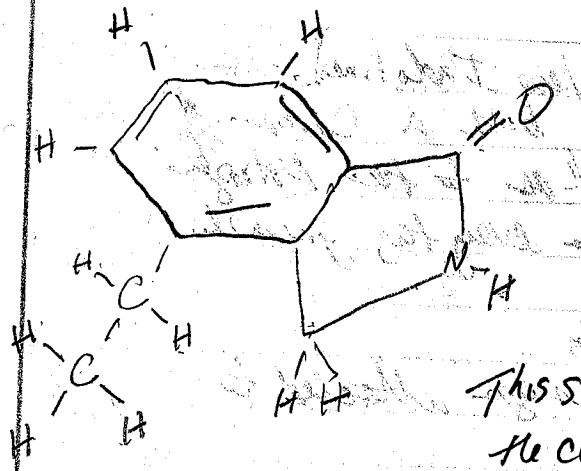
Page 164



but the MW is getting a bit high here. So

upon what basis do you have this? None as far.

Super Cinnamaldehyde



10(12) = 120
1(10) = 10
1(14) = 14
1(1) = 1
161

This seems to be in the class of "Methyloxindole"

So we have maintained the same molecular weight but we have satisfied the functional alkene group and the SOBS criteria.
Now for alkenes.
We need: trans RCH. What does this mean?

This fits ring junction

R=C
|
H ???

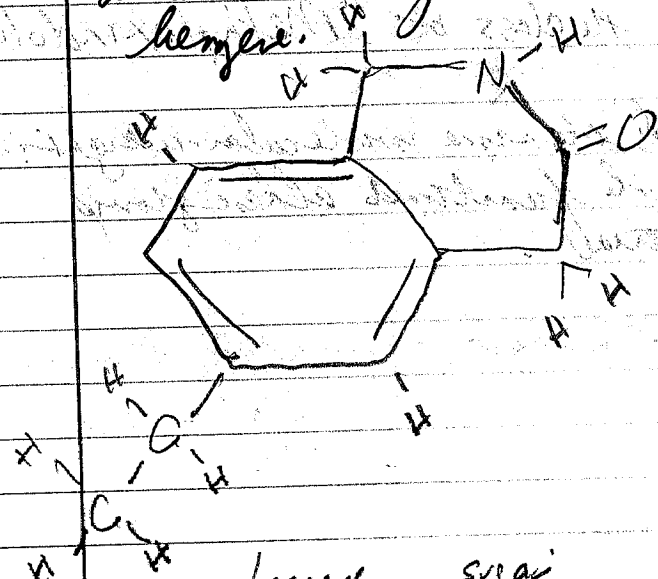
This may be a feasible structure modification.

Let's check on benzene frequency in the SOBS data.

C
mjatkonen@
XS Consultant
group.com

Notice on 7099 (methylene Indoline) a ~~the~~ CH_3 is attached to both a Carbon on the 5 ring as well as to the Nitrogen. This almost accomplishes every thing we need.

29891 is very interesting. Assume we add a sugar attached to benzene.



benzene sugar

this group could go on any free Carbon & could be of different length.

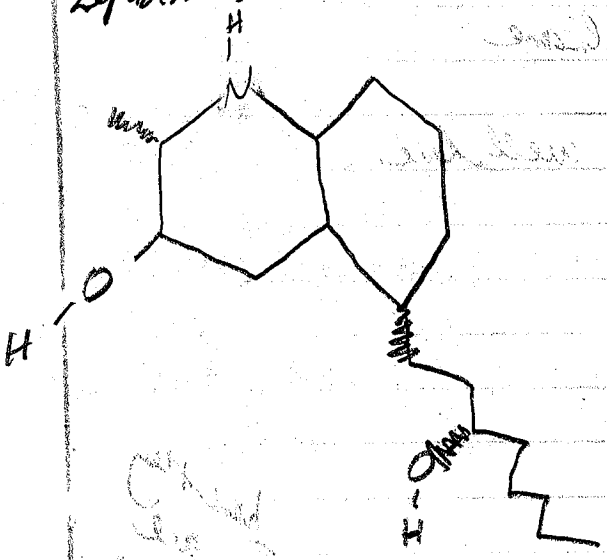
If we have the oxygen attached to the sugar it looks a whole lot more like Ganglioside & Cerebroside.

Page 166

Question. Can we have a C-O single bond in our spectra?

Let look @ our fatty acid candidate

Lepadin



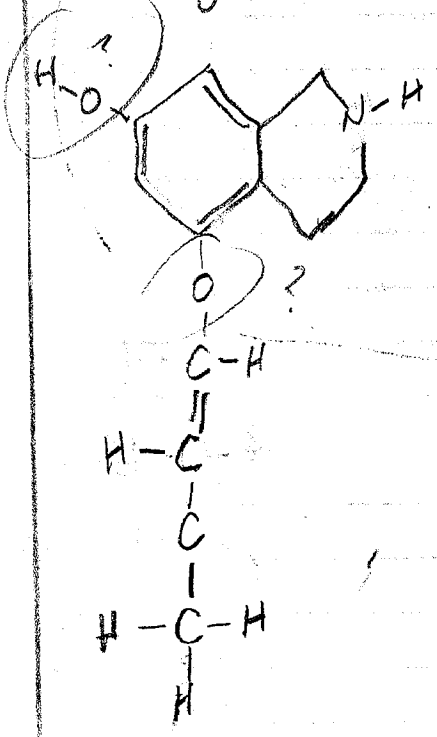
What does mark mean?

So we could search how a
benzene ring attached to
a oxygen
Benzene is the alkene.

Why do we need a C=O
Why not O-C?

What if we had an aromatic Ar-O-R ester?

What if the fatty acid broke off
& left a terminal alkene?

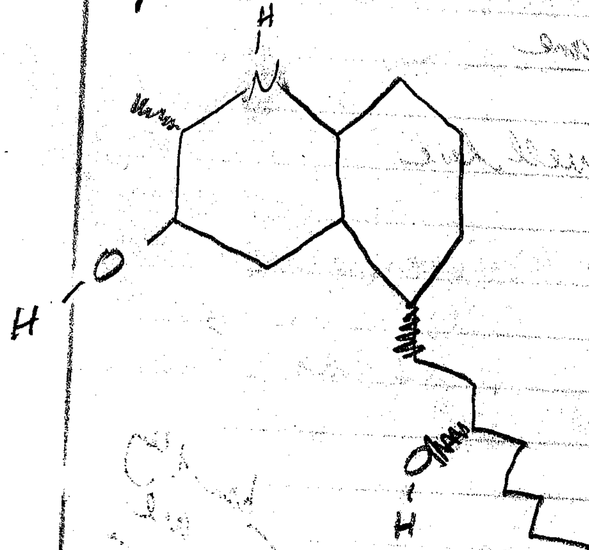


If you had a
hydroxyl group
everything would fit
Phenol? A possibility?

Remember that there are
about 50-60 sphingoloids
in the database so that are
lots of choice & option.

Phenol groups & ester groups
are an activity topic right now.

Let look @ our fatty acid candidate
Lepadin,



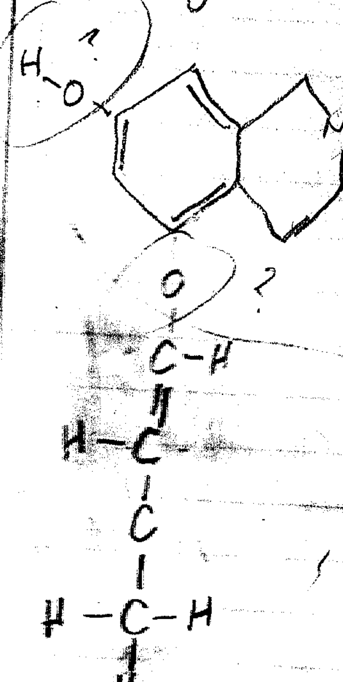
What does mult mean?

So we could easily have a benzene ring attached to a sugar
Benzene is the alkane.

Why do we need a C=O
Why not O-C?

What if we had an aromatic Ar-O-R ester?

What if the fatty acid broke off & left a terminal alkene?



If you had a hydroxyl group everything would fit.
Phenol? A possibility?

Remember that there are about 50-60 sphingoloids in the database so there are lots of choice & option.

Phenol groups & ester groups are an interesting topic right now.

Now we get to move on to IR again.

Not only did we have alkane

$R-CH_2-CH_3$

but an alkene we may well have

trans RCH. what does that mean

$R-C-H$? alkene no less $R=C(H)$?

Stability of alkenes is

$R_2C=CR_2$ More stable

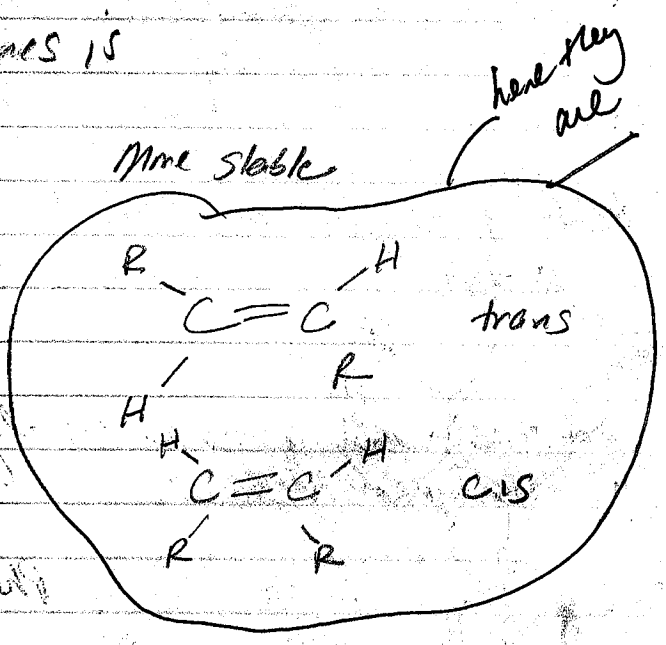
$R_2C=CHR'$

$R_2C=CH_2$

$RCH=CHR$

$RCH=CH_2$

$CH_2=CH_2$ less stable



Unsymmetrical alkenes are less stable than symmetrical

$R_2C=CR_2$ More stable

$R_2C=RH$

$RHC=CHR$ (Trans)

$RHC=CHR$ (Cis)

$RHC=CH_2$

$CH_2=CH_2$ Less Stable

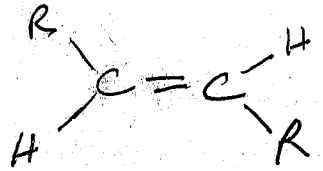
We already know w/ fairly good confidence that we have alkane, alkenes & aromatics

Alkane ~~19%~~ ~~85%~~ 90% Amine - very weak case.
Alkenes ~~87%~~ 87%
Aromatics ~~94%~~ 95%

We also know now that we have both aromatic & aliphatic components.

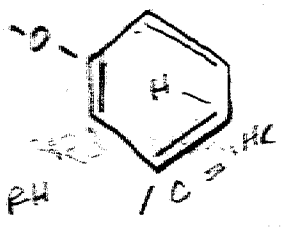
Lets carry on w/ 2960 IR spec
We just picked up on an aromatic methyl by reviewing the Buck Chart. This is very important.

We may have a trans RCH . alkene.
What does that mean.



H means this.

How could this fit into either the benzene ring or the aliphatic chain?



It does not fit well at all into the benzene structure unless benzene can have a trans configuration. I do not believe so.

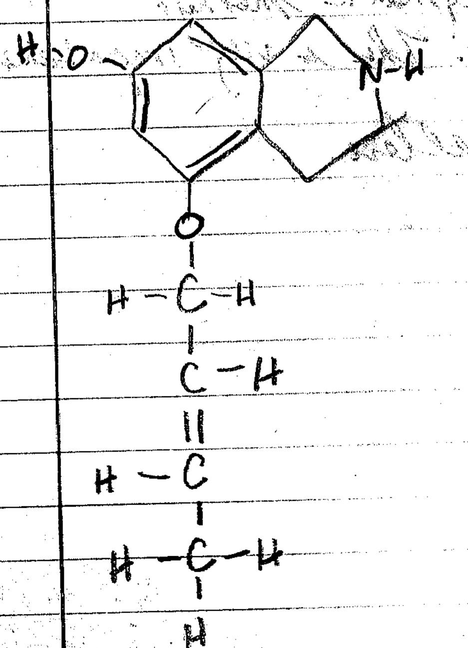
Answer: There is no trans or CH on a benzene ring so they've it has to be on the aliphatic portion.

H is very easy and common on aliphatic chains. Probably more common than CIS I think.

~~So how do you know you have a ring structure attached?~~ Because of 50185 probability. (only so far)

Now we move on to 2920. CH plain & simple

Now Buck brought a methylene into the picture. This means:



I found the ester linkage! p307 Murray India

You are making some breakthroughs on the ester @ 1715 (vs our 1719).

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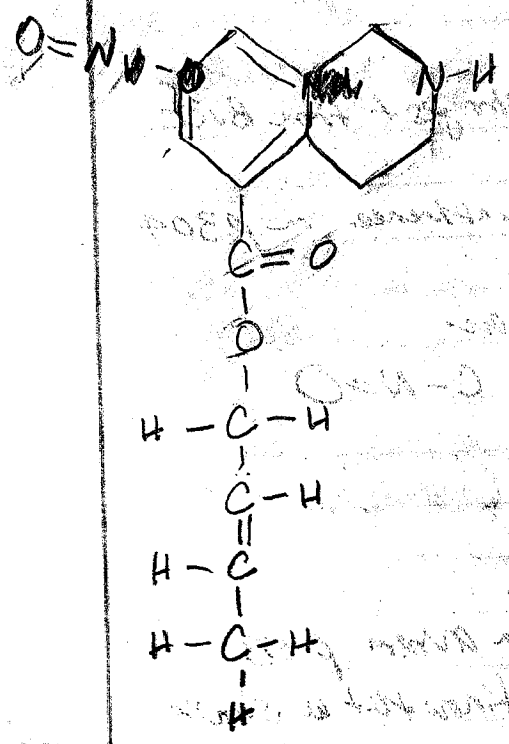
Do we have an ^? NH? OH?



So an ester is starting to shape up.
Keep in mind a phenol and an amine

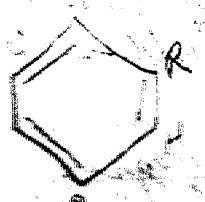
2866 sat to an aromatic methyl
We know that we have both methylene & methyl.

So lets go to 1717
This is ester.

Ester comes in very strong now.
Murray & IR Spec

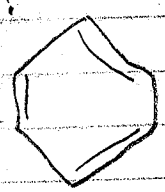
760 is our next strongest peak.

Benzene ring, meta disubstituted comes out strong.
Meta distributed mean.



What if it was flipped?

Phenol?



This matches what we have

R = Carbon, Ester
Aliphatic

Phenol or Aromatic acid targets

Page 171

CG on Buck works next

Let's move to 1495

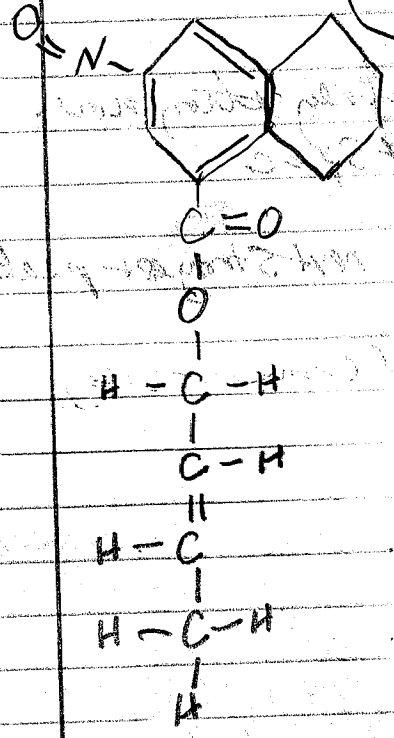
It looks like $Ar-NO_2$ is strongest from Buck.

Murray also indicates this same reference on p304

We know now that we have an aromatic nitroso group $C-N=O$

NH, OH ?

Can it be $O=N-$ NO.



From Avram p313
We know that we should have a para substitution take place.
Should be either OCH_3 or Br (interesting)
this will be in addition to

This is all a maybe.
Koji has 1500 for $C-N=O$
and then could be sufficient.

Page 172

A very important statement in Murray India p386
"Nitration of an aromatic ring does not occur in nature but is particularly important in the laboratory because the nitro substituted product can be reduced by reagent reagents such as Iron to yield $Ar-NH_2$"
Sounds very important.

We must wonder from AVRAM p 313 if the reduction of the frequency from 1500 to 1495 might be reduced by an additional substituent as in table II-112.

So we have a nitroso that in the presence of metallic reagents may form an $Ar-NH_2$.

We have learned that we have a nitroso that may be subject to producing $Ar-NH_2$ The N=O bond will be unstable.

Lets go on.

1610.

Buck: Olefins. Secondary kicks in also
What is an olefin?

It is essentially an alkene, but can occur in a ring also. Can be subject to polymerization.

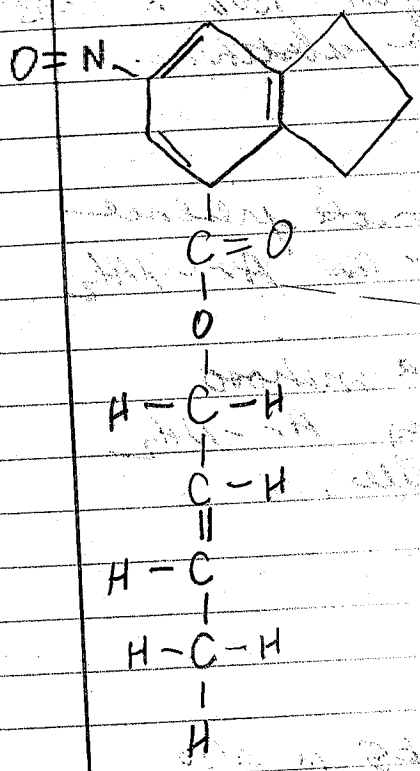
1610 Can also be an amine

Cyclopentene is @ 1611 Avram p 101
See p 89 Murray also.

It is a cyclo-alkene

Can reduce to amines

This is small OK



Very important 1610 strongly indicates olefin & cyclopentene

We also know that it is an olefin

If we search this in pubchem @ 90% we get 14 structures if we set MW to 100-300 960 otherwise

One similar is isobenzofuranone

Watch out what ya call olefin. Olefin really only mean alkene.

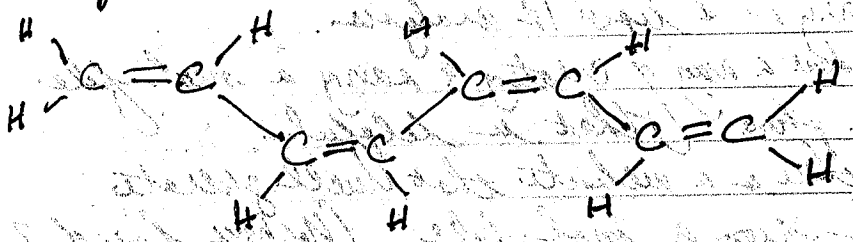
There is also an aliphatic 1611 vibration

so do not assume that it is cyclopentene. Watch this carefully.

Page 174

You may have already determined a 6 carbon structure. Whether or not ya have a sugar is important.

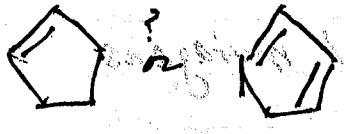
see p 187 Avram. CH_3-C



It says that it is weak. Ours is ~~very strong~~ moderate.

actually Buckle has 1611 under cyclic hydrocarbon after all. w/ secondary also in place.
Then a strong candidate then.

This brings us back to cycl. pentene. p 181
So. is cycls pentene



It is only one double bond & the base.

Jul 26 Sunday

Let's carry on & keep IR analysis.
You now have a way of creating & saving a mol file on your phone. That is helpful.
See if there is a website that will generate smiles from a mol file. (You have 2 but neither works so far)

~~Ethyl nitro fluorene carboxylate~~

Pub Chem has come up w/ 21 matches.
Best no. match is 106864-63
butyl nitro fluorene carboxylate

"mutagenicities induced by nitrofluorene"...

Nitrofluorenes are bacterial mutagens

—

Diospyros

Family Ebenacea

Carotenoid

Indian Medicinal Plants:
An illustrated dictionary by C.P. Khare

An alkyl is an alkane that is missing a hydrogen.

Lets look @ the next peak. $\frac{100 - \text{Peak Height}}{100}$

Lets try 691.

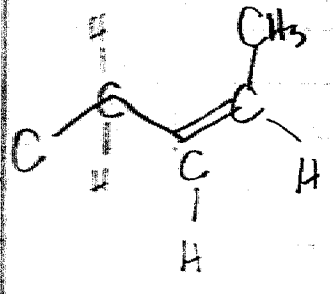
IR Spec 691 alkene
cis-disubstituted (what does this mean)
Benzene ring is in there also. (it means two hydrogens on the same side of the double bond)

Koji 1. alkene
2. Ar-NH_2 (nothing here on IR spec)
3. C-Cl

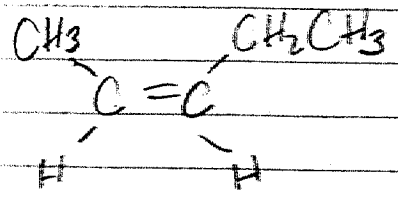
Avram: all of above +
1. Sulfur compounds
2. Quinonoxime

p 179 Pentene-2 @696
Hexene-2 @694

Pentene-2 cis or



there or flipped about the double bond



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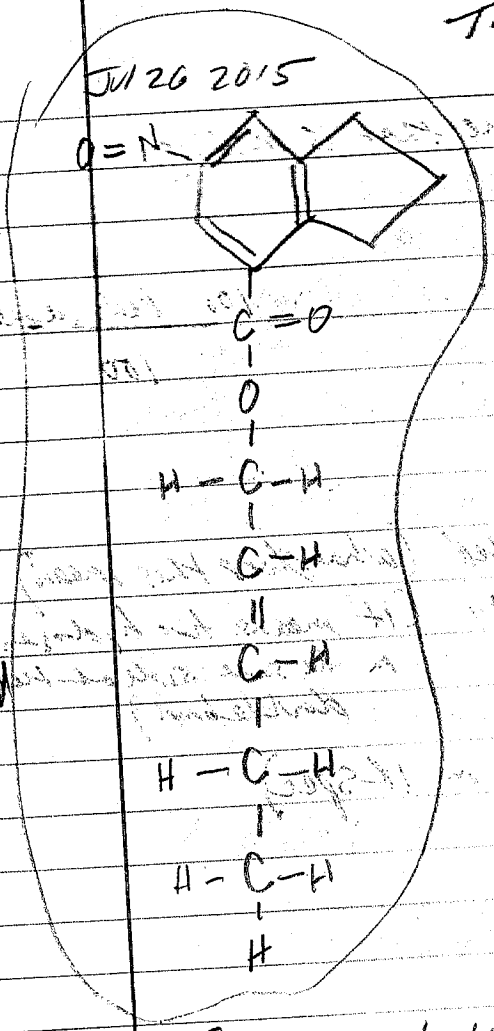
CDB Lipids

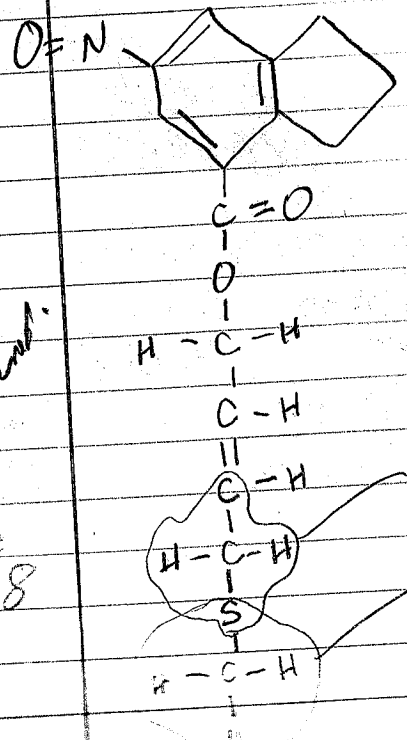
This looks like our latest work.

Jul 26 2015



This remains protonated

I suppose it would be possible for this bond

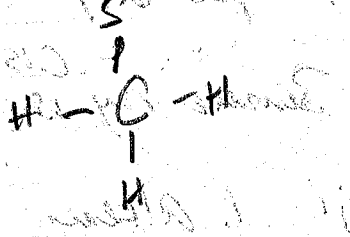


This is not protonated.

but this bond would not be fine as you would expect to see an absorption @ ~ 645

and this bond would be fine @ 691

for sulfur, you would need



Using Silverstein p292

The cone is against the S bond & remains for pentane a hexane

you do not

Page 178

JUL 27 2015 - Monday

We have improved the peak ht weighting system.
The actual peak ht is in now, but an estimate.
Thus a much better. Our probabilities are now:

Alkane 95%
Alkene 79%
Ester 91%
Aromatics 84%
Amine 0%
NO or Nitroso 67%

so Ranked is:

Alkane 95% 87%
Ester 91%
Aromatics 84%
Alkenes 79%

so Ranking is actually:

Ester 91%
Alkane 87%
Aromatics 84%
Alkenes 79%
NO or Nitroso 67%
Amines Ar-NH_2 61%
Nos we Continue & evaluate 69%.
Pentane & Hexane have come out the list.
We want to now consider Ar-NH_2

We need to work out a weighting system of N.
~~N=0~~ N=1 w/ P= 84%
is a system to N=2 w/ P=61%
but multiple scores allow for conformers if in doubt.

but some things only has one peak!

Koji has NH_2 @ 691 (i.e., 650)
an [illegible] of medium intensity & broad. This is not the case at all. Detection can not be justified.

Now we go to AVRAM.
This was not looking great.

Primary amine show two bands. No go.
Secondary amine show one band
(we show one very weak).

OH moved on with this.
w/ Ar-NH-R the freq move to
3430 - 3450.
We do not have this. We have 3406.

This is too weak to justify.
Cutoff is now ~ 65%.

The ~~last~~ next candidate was C-Cl from Koji.
It spec failed this.

Koji 600 - 800
This is very broad & does not mean very much.

p 239 Avram kick in again w/ some meaning
but we have 691 & 742
vs 686 730

It is possible

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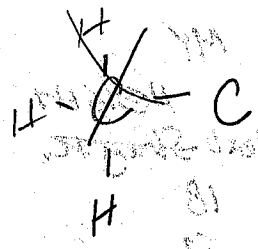
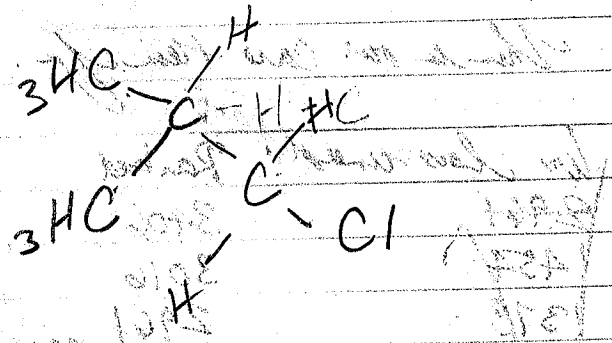
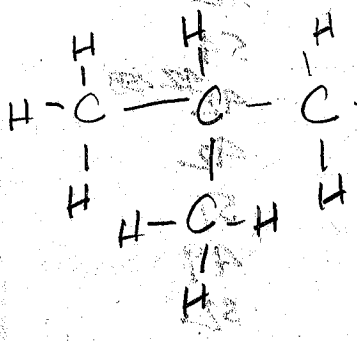
But they still create some problems.

$CH_3-CH-CH_2-Cl$ We really do not have this







This is what you would need & you do not have any thing like this and it is not aliphatic.

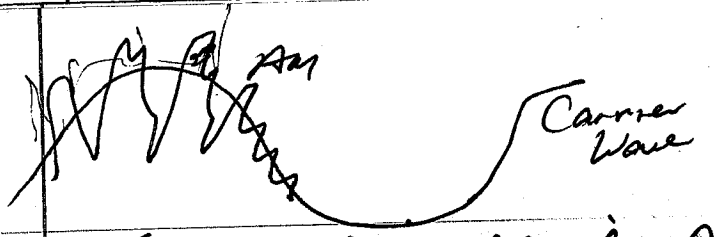
Then the case for a halogen is very weak. Now to the sulfur compound.

Keji is also very broad & that is bad to show.

Auram, however, presents a very interesting case

CH_3-S- occurs at 685-705

How many bonds does sulfur make? 2?



The getnox gurnoxyme Case does not seem especially strong at the time. It is a more exotic & Complicated Structure

Here is our Case then for.

	Ranked	Peak Strength	MY HEIGHT	PH 100-PH
~~2961~~	3406	18		82
✓ 1454	3016	52		~~51~~ 48
✓ 1378	2961 ~2919	54		46 > 42
✓ 2866	2866	42 ~~42.75~~		58
✓ 2961	1717	42		~~58~~
✓ 3016	1495	51		49
✓ 795	1454	49		49
✓ 691	1378	52		60
✓ 1717	795	47		53
✓ 768	768	64		36
✓ 1495	691	50		50
✓ 3406				

So the question now is what would we like to examine that is ≥ 68 that you have missed or conversely what have you missed between 0 and 68

(S21B)
SB1 Norway

NOUN
North Pole?

Let's go over what we have missed so far. 0-68?

	100 - Pkt (lower number is strong)	Peak	
(1)	42	742	save
(4)	68	1218	
(5)	68	1361	OK now
(2)	58	1517	OK now
(3)	63	1610	OK

We have identified 5 sequences in the range that we previously identified (my P.Pt ≤ 64) that we had missed. We must look at them.

They are now ordered & we should look @ them.

742: Benzene ring shows up in IR spec

What is happening in when you get a sequence region addition or decrease the probability which is not right. It should slightly increase it?
OK. Fixed the weighting. Changed from 1.0 to 1/6

Scaled to 95%

					X·√n	Normalized
Now we have						
Alkanes	92%	92%	N = 9	276	100%	
Alkenes	89%	89%	N = 9	267	97%	
Esters	91%	89 90%	89%	N = 3 48 25 3 267 154 180 65	56 91%	
Aromatics	90%	90%	N = 8	255	92%	
NH or NH2	61%	83%	N = 3	144	52%	
NO aromatics	84%	85%	N = 10	269	97%	

Now may have a sulfur !!

Continuing w/ 142

Avram gives us

Alkenes RCH=CHR cis
Arenes
Halogens C-Cl
Sulfur R-S-R
Aromatic Amine
Quinonoxime O_2N-O-R
$ON-O-R$

Then a whole lot more choices than IR spec

Kijn gives us
RNH_2 & $ArNH_2$ T1(3)
S-O T11
C-Cl T13

142 seems to be giving some problems w/ Avram
I cannot find an exact match other than w/ correlation table CIS.

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Notice we have a very strong set of

768 benzene, alkyl halide, alkene
742 benzene, alkyl halide(Cl), alkene
795 benzene, alkene, alkyl halide
691 cis alkene, alkene, benzene, alkyl halide

IR Explainer
768 alkene, phenyl ring substitution, a C-Cl alkyl halide
742 same
795 same

OK You may leave to study this set for now.
Let's go to 1517

Nitro aromatic showing again N-O
Aromatic. IR Spec
This does not match Koji

Has something very interesting
Thiophenes 1520, 1040, & 750~690
Quite a match here.

CDB Lipids: Peaks Chosen

	Ranked:	Reank:
~~2961~~	3016	3016
~~1454~~	2961	2961
~~1378~~	2921	2921
~~2866~~	1717	1717
~~3016~~	~~1517~~ 1610	1610
~~795~~	1517	1517
691	1495	1495
~~1610~~	1454	1454
~~1717~~	1378	1378
~~1218~~	1361	1361
~~1041~~	1218	1218
~~1094~~	1120	1120
~~1120~~	1094	1094
~~3016~~	1041	1041
~~768~~	795	795
~~1495~~	~~742~~ 768	768
~~742~~	742	742
~~1517~~	691	691
~~1361~~		
~~2921~~		

Conclusion: Every peak has been utilized.

Need you here to reffer group question

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Jul 28 2015

There is now a point of consolidation on the lipids that is potentially very important on informational content.

I believe that a reasonable preliminary structural model of the lipids has now been developed.

Review your work at IR pal!

Let's now start to look at the environmental filament.

3279 with a sharp peak.
from Buck, could be acid or a tertiary amine. Secondary amine may be a little fit thru the secondary level

IR spec: Alcohol 3200 3650
Amine 3000-4000
Amine 3300-3500 (may be bad
Alkyne 3300

Koji 3300 (narrow) Alkyne
3200-3400 polymeric OH TS (3)
3300-3500 Amine T1, also C=NH

Avram: The alcohols are just not working.
It is more in the 3600 area.

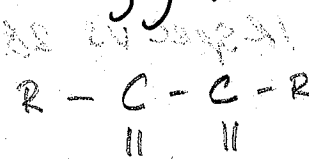
Dioxime is a strong candidate

Avram is racing some interesting candidates.

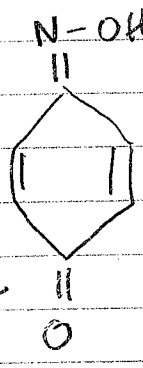
aliphatic
alicyclic
halo
] dioxime

dioximes are apparently also called glyoximes.

also glyoxime



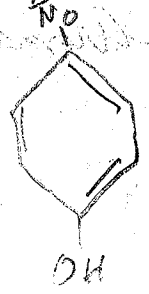
p334-336



"tautomeric" quinone oxime

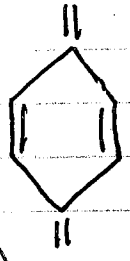
Also quinone oximes are of interest.

e.g. Benzo quinone oxime



Oxime IS $R^1R^2C=N-OH$

Quinone seems to include a benzene ring.



Benzoquinone

Quinone Oxime: $O=C_6H_4=NOH$

Oxime means C=N-OH
There are quinone mono oximes.

From Koji, an aromatic NO is a strong candidate
1300 - 1200 IS intense, not here 1224

Koji & Avram is the pathway
through 3279 & 1224 (Koji, p51!)
1645, 1059 & 972
(maybe even 1576)

1516 Nitro IR Spec matches vs 1520 N-O aromatic

3061 is also an aromatic IR Spec

2919 should be alkane vs 2925

2857 likely also an alkane IR spec vs 2850

500-600 Alkyl Halide IR Spec C-Br

1645 IR Spec is alkene vs 1645

1224 IR spec could be C-O Ether Aromatic

972 also an alkene

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Jul 29 2015

I measured glucose. I measure @ 110
approx 1½ hrs after eating
This looks to be slightly normal

A glucose pill measures 4.4 gms.
We have 50 ml of water. & 0.2 grms dissolved in it

I get a reading of 163 mg/dl

I ~~did~~ diluted by a factor of 2 and I get a
reading of 100

The original solution is now measuring 240
so obviously it was not fully dissolved.
118 when diluted by factor of 2 so

240 w/ 0.2 gms / 50 ml

118 w/ ~ 0.1 gms / 50 ml (118 (2) = 236)

This is all very good so I can create my
own Control solutions!

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The sugars are 4.0 gms = 0.89
out of 4.5 gms total,

So our best estimate of Concentration is $\frac{0.2\,(0.89)}{50\,ml} = \frac{.178\,gms}{100\,ml} \approx \frac{356\,mg}{dL}$

We measure 240
but even error alone could reach ~~445~~ mg/dl so we are all well
w/in range and are not getting a direct readout on solution

However, what if it was salt water?
Would it still measure?
Since it is ready current, not glucose!

Great! Salt water does not work.

So it truly does seem to be measuring glucose.

Powdered Milk Test w/ small portion of a Lactase tablet

	t	Result
	0 min	Lo
now add Lactase		
	1 min	Lo
Δ=5 min	6 min	26 mg/dL marvelous
Δ=4	10 min	46 mg/dL
Δ=10	20 min	90
Δ=10	~~30 min~~ 34 min	164
Δ=6	~~40 min~~ 42.5	113
	50	193
	6061	218
	100	330
	145	355

The experiment is working beautifully.

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$\text{Glucose} = -.037t^2 + 5.92t - 2.55$

$r^2 = .9914$

$\text{Glucose} = -.042t^2 + 6.09t - 3.21$

$r^2 = .994$

You are having a problem getting a reading sometimes
Now this is what you should
1. turn it off and on, insert strip
2. dip quickly and ~~may be~~ hold horizontal
(you have to have the electrodes covered)

~~$= .048t - .084$~~

$G' = -0.48t + 6.09$

$+.084$ $+.048$

$6.09 = 0.48t$ $t = 12.687$ min

@ $t = 12.687$ $G =$

12.5 min

Max Concentration = 217 mg/dL @ t = 72 min

Gluc. Conc $= -.0375t^2 + 5.89t - 2.31$

$r^2 = .995$

$G' = 0$ @ $t = 78.53$ min (max value)

$G(78.53 \text{ min}) = 229$ mg/dL

It has changed by waiting a while.

Now it is

$Conc = -.014t^2 + 4.65t + 5.12$ $r^2 = .992$

t_{max} @ 166 min

$G_{max} = 391$

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Now you should wait till 3 hours!

Now we are @. $Conc = -.016t^2 + 4.80t + 3.61$ $r^2 = .994$

$t_{max} = 150$ min

$G_{max} = 363$

Ok, we are @ the maximum Concentration now.

Jul 29 2005

Very good work w/ the glucose today.
The methods have great potential w/ respect to the monitoring of bacteria metabolism, photosynthesis, and metabolism in general.

Now let's go back to the environmental filament spectrum.

Normalization will be:

Final $$\frac{\%_0 \cdot \sqrt{n}}{\text{Max}(\%_0 \cdot \sqrt{n})} \cdot 0.95$$

We have some kind of error w/ a regression formula that was developed.
It was called "intermediate"

$$\left((1 - \text{AVG}) * 100 - .0954\right) + .9916$$

Ok, it has to do w/ extreme of fingerprint region. Proportionate error increased.

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From IR Spec alone we have the following.

			Score (X Vn)	Normalized *100
Alcohol	~~88~~ 93 ~~79~~%	n=4	185 109	~~80~~% 57% 95
Amine	53%	n=2	75	34%
Amide	84%	n=1	84	38%
Alkyne	79%	n=1	79	36%
Alkane	92%	n=2	130	59%
Alkene	93%	n=5	200	95%
Alkyl Halide	17%	n=1	17	8%
Aromatic	~~90~~ 92%	n=34	~~159~~ 180	~~73%~~ 82%

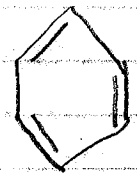
So the score is very poor. It indicates that you have something unusual going on.

Nitro	86%	n=2	122	56%

Your top 3 scores are

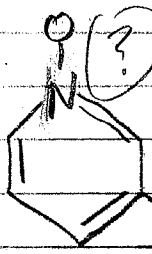
Alkene 95%
Aromatic ~~73%~~ 82%
Alkane 59%
Aromatic Nitro 56%
Polymeric OH 95%

This tells you that you have a benzene ring in the structure.



Now we go to the next source: IR
We know from previous research that on P51 we have a NO compound.

(?) 3 bonds?



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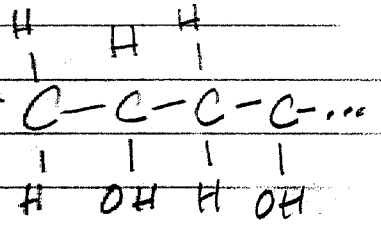
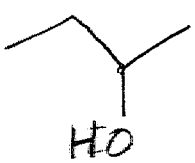


We are headed towards

IR: 3200-3450
Polymeric OH T5(3)

Polyvinyl alcohol? $(C_2H_4O)_x$

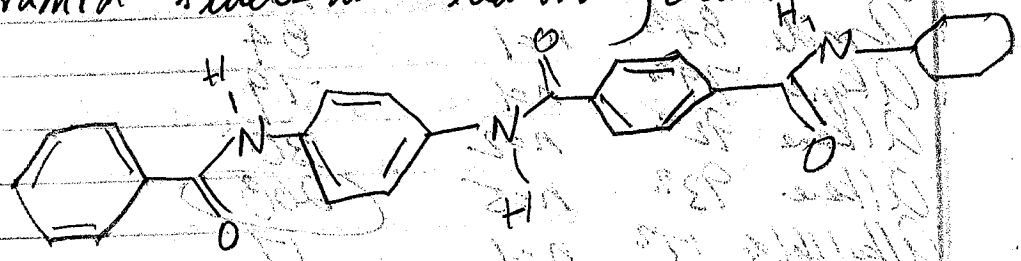


$[CH_2CH(OH)]_n$ a water-soluble synthetic polymer

Benzene - polyvinyl alcohol combination?

" " "

Aramid fibers as a reasonably close match



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July 30 2015

Before we continue w/ the environmental filament, I am Guch is going to help us out a little more on electron configuration graphics and hybridization. He will also help us with acids & bases afterwards and these are both good things.
Spark Chart gives us some info on electronic configuration diagrams and acids & bases also.

Go back to Guch p10
Because of the brevity of Guch, we have intentionally pursued Zumdahl on pp 304-312 because this tells the story much more completely.

Filling is governed by the quantum numbers

n	1, 2, 3, etc	
l	s, p, d, f, etc	(to n-1)
m	from -l to +l	

In combination w/ the use of the periodic table and especially Fig 9.27 on p 321 Zumdahl.

Now let's try oxygen on our own instead of Guch's abbreviated approach.

Of course you can read the configuration from the periodic table but it would be more insightful to follow the style of Guch and to more understand it.

Re quantum numbers

n = size & energy
l = shape
m = orientation
} of orbitals
(I think of M as spin)

Let's take oxygen
n = 1, 2, 3 how far does it go?
It goes to 2.
How do we know this?
It is all governed by the number of electrons and every element is unique & the # is the same as the number of protons & this is all amazing & it comes from the periodic table & to think how elegant the structure of nature is.

So, what you really start with is that Oxygen has 8 electrons. So how do you fill things?

n = 1
(s) l = 0 to n-1 or l = 0
So we have a 1s
m = 0

n = 2
l = 0, 1
(s) p
m = -1, 0, 1

2p ↑↓ ↑ ↑
2s ↑↓
1s ↑↓

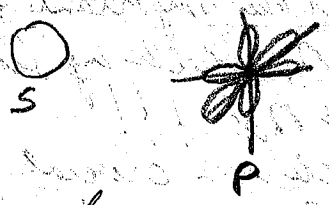
2 electrons
2 electrons

So this is the actual configuration determined from scratch. Pretty good. Now how do you know how many valence electrons...? Because of the outermost layer, which here is n=2 & where there are 6 electrons total & so these are the valence electrons

Now let's analyze & translate (correlate) that picture w/ the Lewis diagram.

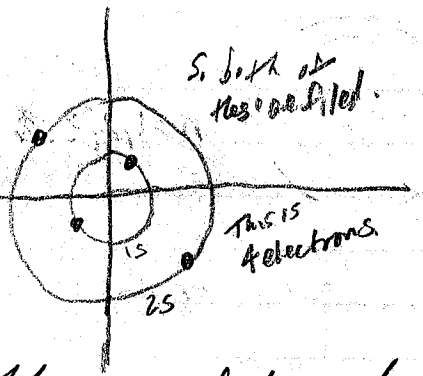
$l=0$ $l=1$ $l=2$ $l=3$

From sparks chart, we can see what s, p, d, f look like.

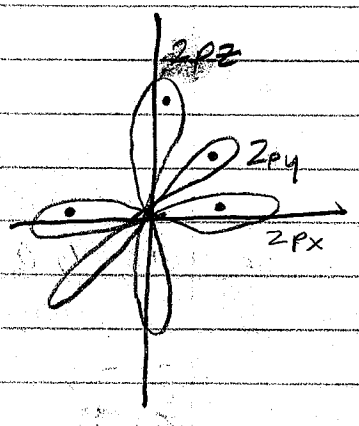


an s holds 2
a p can hold up to 6.

Sodium's last
is a 2s.
This means



now we go to p.
It is a
staged
sequence.
There is no "1p"



The no. of electrons for an element & the intriguing solution by Schrodinger drives everything to construct the orbitals and eventually the valence electron

Now we see the nature of the valence electrons in Oxygen. It's a combination of the 2s (spherical) orbital and 2 1 fully filled p orbital & 2 partially filled p orbitals. These are the valence electrons.
Now in a Lewis diagram you draw only the valence electrons

represents a filled 2s orbital
represents an unfilled p orbital
represents a filled 2p orbital

So two shells are filled & 2 are not

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This would help to explain why Oxygen is so reactive. It seeks stability!!

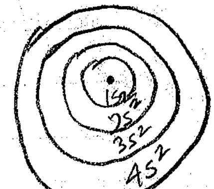
This is very interesting. This helps you to visualize an atom and its reactivity.

Now, for kicks, let's work up iron.
The no of electrons & Schrodinger's equation
determine everything.
Iron: No of electrons = 26
So here we go

A very important qualification
ns fills up before
the same nd !!!
This is a crucial sequence
The periodic table
is your method of
visualizing this.

Σ		
2	2	n = 1
		l = ∅ (up to n-1)
		m = ∅ (-l to +l)
		n = 2
	2	l = ∅ (s)
		m = ∅
		l = 1 (p) (up to n-1)
10	6	m = -1, 0, +1 (-l to l)
		n = 3
	2	l = 0 (s)
		m = ∅
		l = 1 (p)
	6	m = -1, 0, +1
		l = 2 (d) (up to n-1)
28	10	m = -2, -1, ∅, +1, +2

n = 4
l = 0
2 m = ∅
this comes before 3d



= 8 electrons — Σ 8
n = 1, 2, 3, 4

n = 2  $2p_{x,y,z}$ = 6 — 14

n = 3  $3p_{x,y,z}$ = 6 — = 20
6 more to 30

n = 3 $3d^6$ out of 10 = 6 — 26
Remember Aufbau
One in each orbital
before filling
↿⇂ ↿ ↿ ↿ ↿
This is how the d's
of iron look.

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So the configuration is $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^6$

$1s^2 2s^2 3s^2$ ($4s^2$) $2p^6 3p^6$ ($3d^6$) This is Iron.

n $1s^2 2s^2 2p^6 3s^2$ [illegible]

Today the objective was understanding the electronic configuration visually, the shape & sequence of the orbitals

The quantum numbers n
l (to n-1) i.e, S, P, d, f
m from -l to +l

and the corresponding stability of the orbitals

were all very important topics.

Next time we will talk on hybridization & then acids & bases. Such may not be the best again for hybridization — I think a geometry approach will be better than his "rules" because his rules do not seem to work well.
Such is very confusing on the matter.

But Zumdahl was just marvelous w/ my current understanding electronic configuration.

Hybridization will be fun. It will be dependent upon geometry of the molecule at the central atom.

Zumdahl p 389 & 425 are critical pages

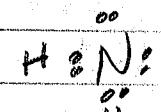
VSEPR & Hybridization

Let's revisit the example in Gucc and determine geometries ourselves.

Zumdahl Chart p 424 shows the end game. The heart of it all seems to be what are called "effective pairs".

Start with NH_3

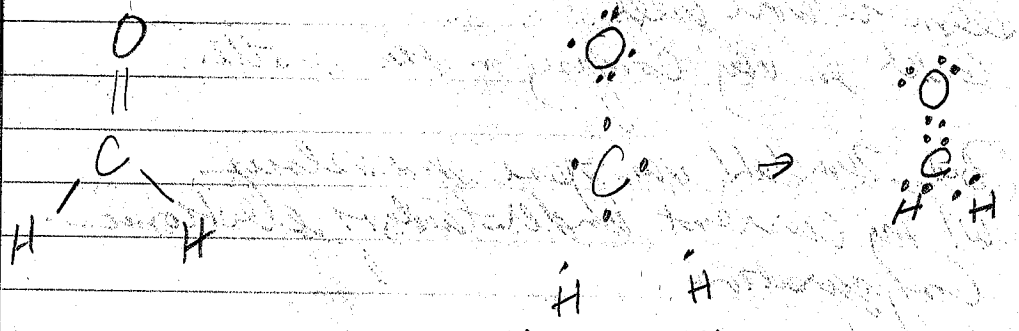
(1)



So what is the geometry? 4 atoms as far from each other as possible this is tetrahedral.

Hydrogen has S
Nitrogen has S & P
So we have hybridization. sp^3 (sum is 4)

(4)



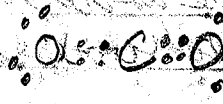
The main idea is that the bonding & the non bonding pairs want to be positioned about an atom as far as possible. Multiple bonds count as 1.

trigonal planar is my assessment. So sp^2 is my assessment

H has S
C has Sp need sp hybridization
O has Sp

(3) $H-C\equiv C-H$

$H-C::C-H$ linear sp

(4) $O=C=O$ 

This is also linear SP

The question of hybridization is not difficult if you can:

1. Draw a Lewis structure
2. Determine the geometry (The bonds and the nonbonding pairs (ie, lone pairs) will be positioned about an atom as far away from one another as possible)
3. The geometry creates "effective pairs", or effective bonds, as what I would call them.
4. The geometry determines the total no of effective bonds. This determines the hybridization the sum of s & p equals this total & S is always 1.

It is indeed a curious process but wonderful to see it unfold.

So today I have grounded myself with

1. Electronic configuration & the stability of an atom
2. The essence of the periodic table whereby each element is incredibly unique as determined by the number of electrons that it has.
3. How to now visualize the electronic configuration of an atom and actually even determine it visually if need be.
4. Re-establish the VSEPR model and how to determine the geometry of a molecule, largely based upon Lewis structures
5. How the hybridization of a atom is determined from the geometry.

Thu was a powerful session & I have to say Guch was a prompter but he was also incomplete.
Guch tells you what you need to know.
Zumdahl actually teaches you & explains what it is that Guch pointed out was important to know.

and Murray is a master of the whole organic chemistry story in detail

GUCH caused me some problems.

Back to the Env. Filament

Lets review this 3279

In Koji p 208 We have something visually that is the most similar thus far.
It is assigned to OH.
Shows a broad, it fits.
This actually looks quite good.

Great, I have normalization into the picture now.

Now we have

Polymeric OH	93%
Amine	34%
Amide	38%
Alkyne	35%
Alkane	58%
Alkene	93%
Alkyl Halide	0%
Aromatic	81%
NO Aromatic	54%
Co Aromatic	34%

Ranked

Polymeric OH	93%
Alkene	93%
Aromatic	81%
Alkane	58%
NO Aromatic	54%
~~Alkyne~~	~~35%~~
Amide	38%
Amine	34%
Co Aromatic	34%
Alkyne	35%
Alkyl Halide	0%

Current:

Polymeric OH	90%
~~Amine~~ Alkene	86%
Aromatic	84%
Alkane	54%
Amide	35%
Alkyne	33%
Amine	31%
Oxime	31%
CO Aromatic	29%
Alkyl Halide	7%

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Jul 31 2015

3279 seems to be pretty strong @ the polymeric OH band.

Primary amine - tertiary is also of interest however.

Amines are just not matching.
But polymeric OH stands, even coming out of the peak. I need to go with it for now.

~~SOBS 12592 looks remarkably close~~

methyl amino pyridinimine hydroiodide
SOBS No 26565
has some similarities

Page 206

Env. Filament SDBS Search

[redacted]

Aug 01 2015 Bass Creek

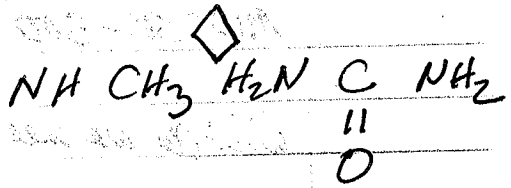
We started an SDBS search. 50 n=2
We are using peaks 60 n= =17
MW 50-300 70% ± 15 n=35

3279 1224 1645 1516 2919 3061 500 +-15 IR

Supplemental are 2857 1059 972

Nos are
25122
26565
34690

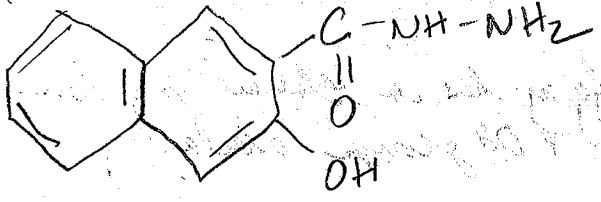
$C_4H_9NCH_4N_2O$



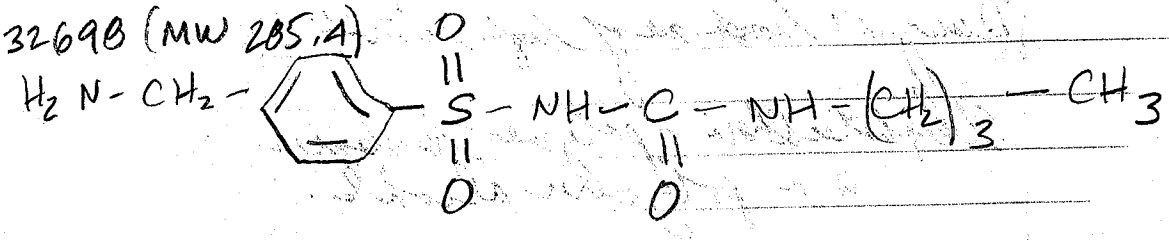
n=2

6893 $C_{11}H_{10}N_2O_2$ hydroxy napthohydrazide
32968 $C_{12}H_{19}N_3O_3S$ aminomethyl phenosulfonyl butylurea

6893 (MW 202.2)



32698 (MW 285.4)



The two searches from SDBS are yielding fascinating results.

Our search criteria was
3279 1224 1645 1516 2919 3061 580
Supplemental 2857 1059 972
Error ± 15
Min Transmittance 50%
MW 50-300

What do we see in these finds?

1. Benzene ring (single & multiple)
2. C=O, C-NH
3. Both NH & NH_2

4. OH group
5. Disulfide bond
6. Aliphatic chain.

What is clarifying here is that we may have both amide & OH groups overlapping.

Disulfide bonds are of high interest.

Aliphatic chain - polymer tendencies & or polymeric alcohols.

Page 208

Lets look @ the case for the C=O bond.

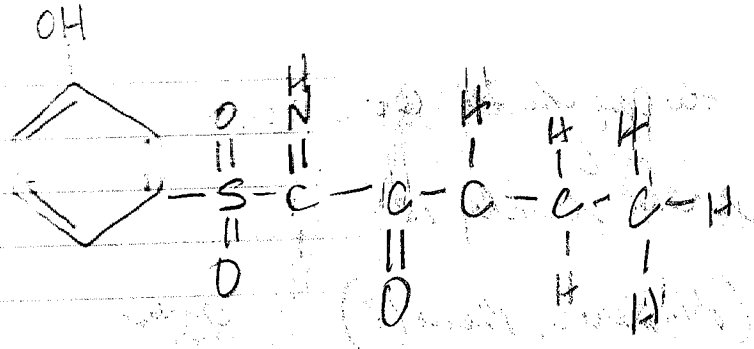
Our current ranky is:

Alcohol (Polymeric, Phenol?)	93% ✓
Amine	29% ✓
Amide	33% ✓
Alkyne	31% ✓
Alkane	51% ✓
Alkene	81% ✓
Oxime	30%
Sulfide-disulfide (Sulfoxide)	74%
Alk Halide	~~42~~ 41%
C-O Aromatic - Ether	28%
N-O Aromatic	47% ✓
Aromatic - NO	80% ✓

So ranked is

Alcohol (Polymeric, Phenol)?	93%
Aromatic - NO(2)	80%
Alkene	81%
Sulfoxide, disulfide	74%
Alkane	51%
Amine	C=NH 72%
Amide	33%
Alkyne	53% ~~31%~~
~~Amine~~	~~29%~~
Oxime appears to be a -N=OH	30%

Check these thoroughly

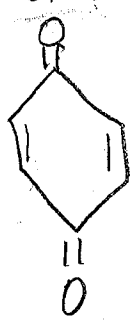


First proposed model of environmental filament.
Minimum Configuration

What is an oxime?

Koji 1605 extended quinone

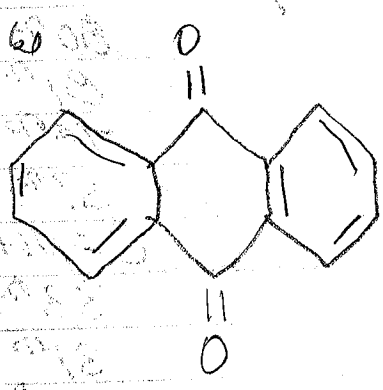
quinone is



quinone

hydroquinone

Could be



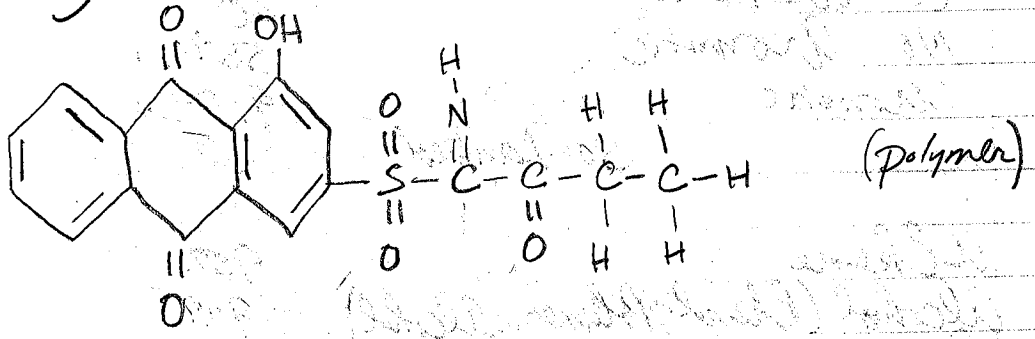
Polycyclic quinone occur in some bacteria fungi.

an OXY PAH
polycyclic aromatic hydrocarbons

they are toxic

Organisms closely related to Sphingomonas were the most predominant

they are oxidants & electrophiles



Current model of Env. Filament

Polymeric alcohol
aromatic polymer

Now let's hurry it along to the picture.
Start 4/3279

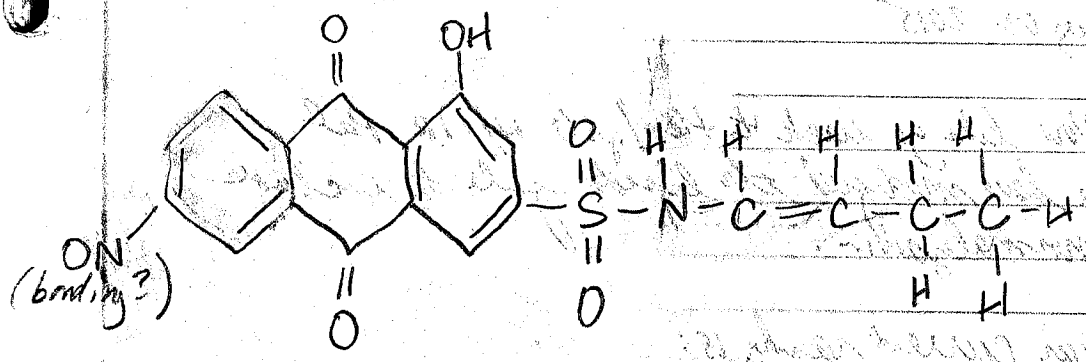
With IR Pal included, the ratings are:

Alcohol (Phenols, Polymeric)	92% ✓
Amine NH	66% ✓
Amide	47% ✓
Alkyne	47% ✓
Alkane	58% ✓
Alkene	95% ✓
Oxime	34%
Sulfoxide, Disulfoxide	76% ✓
Alkyl Halide	47% ✓
CO Aromatic	20%
No Aromatic	55% ✓
Aromatic	91% ✓

So Ranked:

Alkene	95%
Alcohol (Phenol, Polymeric Alcohol)	92%
Aromatic	91%
Sulfoxide	76%
Amine NH	66%
Alkane	58%
No Aromatic	55%
Amide, Alkyne, Alkyl Halide	47%
Co Aromatic	20%

Env. Filament Project



Current Model w/ IR Pal included Jul 01 2015

Name is

~~Dioxo dihydro anthracene sulfonamide~~

~~Pub Chem has a structure very similar @ the 95% level.~~

~~name is~~

~~butyl dioxoanthracene sulfonamide~~

~~the Pub Chem No is 3089312~~

~~There are only 5 Compounds @ the 80% level~~

yes 3089312

butyl dioxoanthracene sulfonamide

also called anthraquinone (without the sulfonamide)

anthraquinone sulfonamides

are involved with "Stabilizing triplex DNA"

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[redacted]

Aug 02 2015

Now lets go back to the lipids w/ IR Pal
We have modified the lipids file to include normalization.

Our current ranks is:

Alkane	92nd 03
Alkene	~~89th~~ 85th
Ester	~~84th~~ 86th
Aromatics	~~85th~~ 81st
Amine	~~40th~~ 43
Nitro Aromatic	~~90th~~ 95th

The looks very good now. It looks like very reliable information.

Now lets go to proteins.

[redacted]

Aug 04 2015

Lab:

[redacted]

1. Iron into Lipids?
2. Stain IR

The idea of Fe^{+2} dissolved in the lipids did not work because $Fe^{+2}SO_4^{-2}$ is not soluble in
1. the lipids
2. ethanol
3. n Isopropanol.

I do not know how to get at a variable to the lipids.
Soap?

I did hemoglobin test.
It appears to me to be at most 50%. I think
Close to 45%.
Should be a 40%. So it does look
Close but maybe a little low.

I measure 47%. This is just about right.
The test worked.

IR Skin test failed.

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Saliva?

(centrifuged) gives a better result than jelled blood cells do.

Urine, mostly evaporated, surprisingly Gives a better spectrum than urine paste.

Aug 04 2015
I have another protein plot. It looks very usable.
We need to do some averaging on the peaks

We have a 3519 that is unused.
Amine & Alcohol are Candidates.

Next we have 3357 + 3363 ⇒ 3360

Next is 3220 + 3240 ⇒ 3230

Next is 3052 + 3090 ⇒ 3071

Next is 2913 + 2920 = 2917

Next is 2760 Could be amine again
Must not have aldehydes in
the area. Not recorded.

Next 1594 + 1630 = 1612

[redacted]

[redacted]

Aug 05 2015

OK, for today, where are we?

1. Capillary tube & Kates blood.
   To extract we need to sacrifice tubes.
   Can we improve?

2. Lipids, hemoglobin & soap?

You have learned some very important things about scanning today, esp w/ blood & the samples.

1. You do not have to scan everything, especially if water is involved in the problem.

2. A scan of blood from 2200 - 600 is much more useful than trying to scan the entire range.

3. The background must correspond w/ the partial scan

4. With salt crystals, at least (I cannot say about soil yet) the background must be left as the original file. Alternately the files only caused major problems.

5. The software always generates an error w/ a partial scan but it is not terminal.

6. A scan of 10 relative to a normal background presents big garbage.

7. You end up getting a very good blood serum scan (Katie) w/
1. 2200 - 600
2. normal background removal, no attenuation in any original file.
3. some smoothing
4. scale to 100 as usual.

5. Combination w/ ATR may indeed be fruitful.

What we are doing here is contextually different spectra.

You see numerous opportunities for error,

Many of our sample types are not applicable or amenable w/ very weak signals. Welcome to reality.

You do not need to scan the whole thing, especially if water is involved. You can bypass water & get a more selective scan on more specific features.

You still have not had lectures started at the benefits of ATR.

Have you run a complete hunt. Why?

Aug 07 2015

[redacted]

2. Glucose monitoring of culture is a very interesting topic.

Culture started on Jun 16 205

30 ml H_2O
4 drops CDB (Use powder also)
.10 Grams Fe+2
H_2O_2 6 drops
Sugar 0.25 gms

Measurement of Glucose of existing 30 day old culture

271 mg/dL
this is quite high.

Regular sugar in water is Lo!

This is very Good.

Fe+2, Sugar, Water, CDB (No filament production)
measure 394. Excellent

Need
1. Scale
2. Petri dishes
3. Sugar
4. Iron
5. CDB
6. H_2O_2
7. Camera
8. pipettes
9. LED scope
10. Glucose Equipment
11. Vials instead?

Glucose

Notice, flat after 30 days

394 — The Culture w/ COB, Sugar, Water & Fe+2 only produces CBB Coccus form

271 — Culture w/ COB, Sugar, Water, Fe+2 & H_2O_2 produces filament & Coccus

---

We appear to have an important Catalytic reaction (assume Catalase) reaction occurring w/ the Env. Filament when subjected to $FeSO_4$ (+2) and H_2O_2. It appears to generate protein detectable w/ IR

---

after 22 hrs:

(D2) : Glucose $\cong .39t^2 - 8.11t + 88.3$

$G' = 0.78t - 8.11$

min $G' = 10.4$ hrs

(394) Glucose $\cong 1.29t + 40.3$

The peroxide group is rising steadily. The non peroxide group decreased to a minimum and now is rising again

Fe+2 Sugar CDB H_2O (1) | Same as #1 (2) | Fe+2 Sugar CDB H_2O_2 H_2O (3) | Same as #3 (4)

Elapsed Time hr — Start Test @ 2000 08-07-15

Elapsed Time hr	(1)	Δ	(2)	Δ	(3)	Δ	(4)	Δ
0	85		47		Lo <20		39	
0.5	100	15	85	38	25	15	47	8
1.0	96	−4	85	0	49	24	31	−16
2.0	96	0	88	3	54	+5	56	+25
4.0	62	−34	34	−54	62	+8	50	−6
22.5	96	+36	116	+82	70	+8	63	+13

@ 4' / 22.5 — .188 2.05 1.64 .930 x=.645

We are getting an avg change in both groups of ~1.76 mg/hr

Production should increase @ some pt to ~4 mg/hr

+1.5=24.0 = 2000 on 08-08-15

+18.5 = 1430 on 08-09-15 = 38.5 hrs

38.5 97 94 76 58

a = 0.59 mg/hr $\bar{X}$=16.8mg/day a=0.80

24-14.5= 9.5hrs. 38.5+9.5 = 48hrs. +15.5 = 63.5hrs

~~63.5~~ 2000 on 08 07 15 Start. Date Now is 1130 on 08 10 15

63.5 = 1130 MT on 08-10-15

63.5 97 a=.06 20 80 a=.68 85

114 = 1400 MT on 08-12-15

114 109 22 107 123

a=−.13 a=.64

142 = 1800 MT on 08-13-15

142 101 123 132 111

? = 1900 MT on 08-15-15

71 (red filaments have formed) 101 174 144

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Ok, let's move on.

I would really like to be able to get a skin culture. How?

Saliva works very well.

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Aug 10 2015

GC - Atmosphere!

CO_2 peak @ 2.30 min

Δ = 1.75 min

N/O_2 peak @ 0.55 min

CO_2 peak .226 mV
− .064 mV base
Δ = .162

Δt = 2.64 min − 2.06 min = .58 min

.5(b.h) = .5(.162).58 = .047

N_2O − Δt = 0.97 − 0.43 = .54

Δh = 590 mV − .104 = 589.9
.5(b.h) = .5(.54)(589.9) = 159.27

$\frac{.047}{159.27}$ = .000295 = 295 ppm } excellent work CO_2 concentration

What causes O_2 & N_2 to merge?
What causes baseline drift?

Avg successful experiment. 3% CO_2 available breathing rate.

Aug 10 2015 Atmospheric Air

Undetected CO_2 peak

$\Delta h = .224 - .07 = .154$
$\Delta b = 2.66 - 2.06 = .60$
$A = .5(.154).60 = .046$

$N2O2 = 5471.4$
$CO2 = .046$

CO_2 toxicity is a very interesting topic.

% CO_2 PPM =

N_2: $\Delta h = 582.3 - .107 = 582.2$
$\Delta b = 1.18 - 0.41 = .77$
$A = .5(582.2)(.77) = 224.15$

CO_2 PPM = $\frac{.046}{224.15}$ = 205 PPM OK = .02%

Balloon CO_2: $\frac{249.2}{8043.4}$ = 30981 ppm?

N_2O_2

N_2O_2 $\Delta h = 819.4 + .069 = 819.5$
$\Delta b = 1.12 - .42 = .70$
$A = .5(819.5)(.70) = 286.82$

Air Peak = .0 DB min

CO_2: $\Delta h = 12.909 + .202 = 13.111$
$\Delta b = 2.78 - 2.01 = .77$
$A = .5(13.111)(.77) = 5.05$

$\frac{5.05}{286.82 + 5.05}(1E6) = 17607$ ppm = 1.76%

Holding my breath / exhale into balloon

Factor of 88%

Next we are running the same test @ 60° vs 80°.

It definitely made a difference & slowed things down.

Area % = 252.4 / 5705.1 (1E6) = 44236 ppm
= 4.42%

These Peak simple values are off by a factor of 2.

$\Delta h\ O_2NO_2$ = 611.6 − (−.18)
$\Delta s\ O_2NO_2$ .99 − .43

$\Delta h\ CO_2$ 9.58 − (−.53)
$\Delta s\ CO_2$ 4.04 − 3.08

% O_2 = 2.75%

So it came out quite a bit higher.
Than the first set.
All that you changed was the temperature.

Avg = (1.73 + 2.75)/2 = 2.24% = 22,400 ppm

Roughly a 100 time greater than normal.

Aug 12 2015

GC

1. You have learned a lot about cleaning the instrument. You had some major contamination in there.

Multiple extended runs @ 220° were required. Double bake outs on filter were required.

It is performing like a champ now. And it has stabilized.

2. Next, there should seldom be a need to ramp up. You can see if it is still stable w/ ramping later.

3. For now, run a survey @ high temp (220) to make sure nothing gets stuck in the column.

4. Then lower the run to about 150°. Increased sensitivity results.

5. Then lower the run to ~80° if needed.

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Increased temps & long time means
a Column that stays Clear &
ya get the big picture & lower sensitivity

Lower temps means greate sensitivity.
Do not go that until ya have
the big picture & hard and the
instrument remain stable.

Changing the oven temp decrease stability.

Use	220°	~~15 min~~	20 min
	150°	~~12 min~~	15 min
	90°	~~90 min~~	12 min
	60°	~~6 min~~	10 ~~8~~ min

acetone ↑

← Deuterated alcohol

In addition to

O_2N_2 @ 0.6 min

CO_2 @ 3 min

Something very small @ ~7 min

We determine CO_2 tonight @ 300 ppm.
Looks very good.

We determine exhaled (held breath) CO_2 concentration @ 2.17%

Surprisingly close to the average of yesterdays work.

I would say very good work and your machine is clean.

Page 234

Now how about denatured alcohol again?

@ 220 looks like 2 peaks w/in one minute

Something happened @ 10 min that is

very big & that is our surprise.

We get a very broad peak.
somewhat like we saw in the cleanup air.

Seems like it needs to be @ a high temperature.

It is, however, only about 4mV

Clean it out again. Higher temp possible?

GC work Aug 12 2015

I first found peak of MEK.
Then refined to work first (@ 50°C).

Next I mixed in acetone. Still only have one peak.
Let's look @ Δt for both files & see if the peaks are the same.

MEK by itself $r_2 = 0.69$ min

Air peak @ 0.13
Second air peak? 0.16

2nd file

$r_2 = 0.66$

Air peak 1 @ 0.10
Air peak 2 @ 0.15

These values are starting close.

Lets try Xylene.
Xylene seems to have the same kind of peak. How and why?

$r_2 = 0.67$

Air peak = 0.11

Next, you have Xylene
w/ 1 & 3 drops CDS Lipids!
Did not work.

We had gone back to gas analyzer.

We used a propane air mix.
A very highly successful result.

We ended up w/ 4 peaks, not 3
which I believe actually represents 5 gases.

~~N_2O_2~~	TC	~Ret. Time	
N_2	.0243	.61	
O_2	.0246	.64	
Propane	~~.0202~~ ? .0202		3.39
CO_2	.0144	4.53	
Unknown Gas	?	7.44	
~~Propane~~	~~.0202~~	~~7.44~~	

Unknown Gas?

$r^2 = .84$

$y = .0226 - 4.037E\text{-}3 \ln(\text{Retention time})$

Power

$y = .\frac{.0267}{\cancel{.0223}} e^{-.118 \cdot R}$

Butane is 0.014 so it is not linear

Must depend on the concentration also

We are starting to see why some gases do not separate & Condense into one!

It depends on the thermal Conductivity TC
It must be different!

Notice N_2 & O_2 have the same
@ room temperature
N_2 = .0243 This is why you cannot
O_2 = .0246 separate it.

Helium is very high @ 0.170

CO_2 is 0.0144 and generally pretty low.
Cl_2 is lower
You could probably capture baking soda in a test tube like you did for propane.

Ethanol is .169 so they are very close
Acetone is .161
Propanol is .154
Methanol is .200

} This is why alcohols are hard to separate.

Water is 0.61

Helium is .141

So it seems to me the Concentration, the thermal Conductivity are major factors.

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I have now succeeded very well w/ the

1. Room air
2. Exhaled air & held breath
3. Propane from a canister mixed w/ room air
4. CO_2 captured in a balloon from baking soda & vinegar

(!) You learned that propane is a mixture of at least 2 gases.

(!) You have learned that baking soda & vinegar produce another gas! Namely CO_2

Next I am doing car exhaust.

Significant Limitations to GC

Aug 14 2015

Webinar on Sample Prep in GC

1. Sample must be volatile (40-50 torr @ ~300°C) 350°C
2. Low molecular weight (< 800)
3. Must be a clean sample
   (no urine, blood, rocks, sticks, stones, wastewater, etc)
   liquid - liquid extraction - what is this?
   solid phase extraction
4. Liquids, gases, solids dissolved in liquids

Liquid liquid extraction is bringing two liquids together to transfer soluble substance from one liquid to another. (usually H_2O & org. solvent)
It is an extraction of a substance from one liquid into another.
The two solutions are immiscible.

SPE is Solid Phase Extraction
Non Polar against Polar is a common method.

"Log P" tells you how polar something is.

log P < 1.5 Very Polar

> 1.5 < 4 Moderate Polarity

> 4 Non polar

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You make derivative if it does not meet the GC criteria.

(Remove hydrogen bonding sites & it makes it more volatile)

You need a 5 Angstrom filter in your gas line.

Watch for injecting air into TCD GC it seems it may cause oxidation of the filaments

How does the compare to sandwich injection method.

SPME Solid Phase Microextraction

do the headspace idea did not work yet.

Aug 14 2015

GC Practice

I have mixed Xylene, MEK, Acetone & then I have extracted the gas only.

I had some interesting results. I had peaks @

45c .05 min (not sure)

45c .08 min (definite) & it looks like it could be two different peaks

45°C 9.50 very strong

6.55 very small looks like CO_2?

150°C 14.79 Sharp strong peak but very small

Repeat under survey mode:

			Use Air Next
?	.06	.05	.06
H_2O_2	0.56	0.55 (This could be 2 peaks combined)	0.54
CO_2	4.79	4.12	4.76
	8.85?	8.36	

Page 242

Re zero causes a distortion in the graph.

Aug 15 2015

I think you are now understanding why certain materials are not working well i.e. solvents, in the TCD GC instrument.

TC & Helium seems to work fine.
TC + Helium seems to be a reliable issue.

Lets work w/ Xylene
TC of Xylene is: Ø.131
vs Helium @ Ø.143

This should make it inherently difficult.
We also see that we have air in the syringe every time we inject it.

It does appear that we end up with an air peak

And not by much. It is also interesting that we have a steady decline in the baseline.

@ 150°C

My own guess is that we cannot adequately resolve these conditions.
Something very minor did happen between 3-4 min but I do not think that it is reliable right now.
~ 3.2 min
~ ~~5.0 min~~ 4.2
~ ~~7.4 min~~ 7.8

We can also try w/ increased current.

Everything you are detecting is w/in 1.0 mV

Our peak ended seem to be @ 0.56 min as before. The first peak is @ 0.09 also as before.

Current now up to 120 mA.

We do have some slope breaks occurring.

One is at 6 min
11.3 min to another.

The could mean we have something. S-13

We have a theory that you might be detecting something @ ~10.7 min.

Method:
1. Zoom in on slope break area
2. Fit a polynomial
3. Differentiate it
4. Find the zero point

Page 244

Let's see if this replicates

RUN 4

Notice that we once again have a decline in the baseline. The slope does not start breaking until about 14 to 15 min or so around.

Let's run it 20 min @ 100° 120mA
Bake out @ the end.

Let's go to 80° instead.

Very clean air peak.

Nice steady decline in baseline again.

False

Must analyze. We have a very sharp negative peak @ ~ 2.6 min.
Very digestive.

Vs 60°C @ 120mA isothermal

Something else very small has happened @ ~ 7.2 7.1

Repeating.

False alarm. We had flipped the breakpoint switch and it created a false peak. Do not do this during a run.

With maya smoothing, we'll establish a peak @ 6.1! Let's repeat

Repeat again @ 80°C.

Nice ox peak. Steady baseline.

There does indeed seem to be a repeat taly place.

Circa 6.6

So we have 7.1, 6.1, 6.6 → $\bar{X}$ = 6.6

We may have deducted a xylene peak. Next we will dry it to 60°C.

Olympic smoothing is best. Window = 10
Iterations = 10, order = 2

Now @ 60°C 120mA 20min
Baseline decrease again. I will assume that stabilization will be required.
The baseline is flattening to some degree after 4 min.
Baseline has flattened nicely after 6 min.

There is a peak @ ~~7 min~~ 6 min.
There may be another @ 10.
Baseline requires stabilization to determine.

Repeat it.

Repeat @ 60° 120 min 28 min.

Baseline is stabilizing.

It appears that the lowest, but absolutely necessary suppression temperature, should be used to increase resolution @ the higher current level if need be.

The run really does not look like it worth. The best run seems to be @ 80°C

The boiling point of xylene is about 140°C so the more perfect sense that you should be @ 80°C vs 60°C.

You cannot go so low as to not volatilize the sample.

Now let's add COB gain.

The baseline has now shifted w/ upward bias. This says to me that as stabilizer, an increase in temperature increases the baseline bias, a decrease in temp decreases the bias.

Something small may have happened around 1.25 min.
The baseline is levelled off after ~ 5 min.
No useful data results.

Repeat @ 60°C
Baseline is more level now.
Superb baseline.

No results visible.

No so back to Xylene

Repeated again @ 60°
Baseline very stable. There are no repeating results.

Conclusion: You can not identify Xylene.

Notes

1

Culture #1 has red filaments forming now. #2 No filaments.

(4)

H_2O_2 vs Control Cultures

*

Day No	Date	Time	No H_2O_2 (5) 1	X	2	H_2O_2 (6) 3	X	4
7.83	08-07	2000	85	66	47	15	27	39
7.85		2030	100	92.5	85	25	20	15
7.88		2100	96	90.5	85	49	36.5	24
7.92		2200	96	92	88	54	29.5	5
8.00	08-08	0000	62	48	34	62	56	50
8.94		2230	96	106	116	70	66.5	63
9.60	08-09	1430	97	95.5	94	76	67	58
10.48	08-10	1130	97	62.5	28	80	82.5	85
12.58	08-12	1400	109	65.5	22	107	115	123
13.75	08-13	1800	101	112	123	132	121.5	111
15.79	08-15	1900	71	86	101	174	159	144
25.46	08-25	1100	107	98	90	201	(195)	189

$\bar{X}$ Cultures 1 & 2: $m = 1.20$ $r^2 = .03$ No H_2O_2

$\bar{X}$ Cultures 3 & 4 $m = 15.65$ $r^2 = 0.95$ H_2O_2

29.71	08-29	1700	115	(111)	107	243	(218)	194

$\bar{X}$ #1 & 2 $m = 1.24$ $r^2 = .19$

$\bar{X}$ 3 & 4 $m = 8.71$ $r^2 = .90$ 7 fold increase in rate

Page 250

Trout Creek Trip Aug 16 2015

There is no need to carry the culture supplies or the microscope on this trip. This simplifies the cargo considerably.

You have enough IR Plots & books on GC to occupy you completely so again this simplifies the cargo.

Aug 16 2015

Blood Serum plot CEC.
Cohn supernt. It is definitely important to use a fresh background spectrum.

GC Watt a Glycerol 180°C
~~13.6~~ min something has happened 13.95 min
w/ a major trail. Magnitude 41 mV
There is only one peak up front, this is interesting.
It suggests the first peak has been the peak & the second large peak has been the solvent peak.

Repeat w/ H_2O only.

A major right tailed peak occurs @ 10.50 min
Magnitude is 70 mV
Did glycerine shift it?

Page 254

Repeat

Same result. 10.47
This means we can detect water.
Does it cause harm to the column?

So now the obvious question is what if we mix ~~alcohol~~ acetone & water?

The tail, incidentally clean after about 30 min.

GOT IT!

A solvent and water have now been detected.

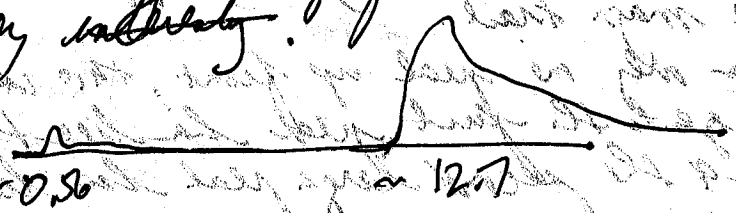
You could next determine thresholds.

You mixed acetone and water.

Acetone is near the 0.56

Water delayed itself from 10.5 to ~ 12.7 min

Very ~~calibrated~~.



Acetone + Water

We have now separated a miscible solvent within water. This is great. This means that all those times you have been picking up the solvent & the air peak is up front. This opens up some possibilities.

You can think now about mixing things w/ a solvent & see if you can detect them. You have done just by such a thing w/ water now. You did not have pure [illegible] w/ the lipids. I wonder how you determine thermal conductivity?

Page 256

Aug 18 2015 Tues

1. We have looked @ [redacted] Sand
2. We have a new history book, which is really quite interesting.
3. We probably need to summarize where we are in the lab work and how to think about where we are headed.
   You have to previous summary of the OR trip which should be evaluated for it's application.
4. You brought all the chromatography books & these actually getting very interesting.
   You have now separated several gases and a solvent - water mix. You see some of the difficulties, but nonetheless, characteristics of water.
5. You have your conceptual math book and your calculator - lots of opportunities here.
6. You have the R book and a stat pack of some.
7. You have a clear new notebook dedicated.
8. You have your IR books - actually very enjoyable reading
9. You have your IR plots & data - there is no end to that study
10. You have your dulcimer & music books.
11. You have some magazines (quite a few)
12. You have organic chem lab books (2) and procedures to learn about.
13. We have Environmental Chemistry
14. We have dissects of a PS.

What struck you funny here?

Topics that immediately come to the forefront are
ALL OF THEM!

Nevertheless,
Chromatography is eager
Lab Procedure, esp w/ Chromatography are eager
IR is fun to no end
Planning the textbook is wacky
Paper a Chromatography are unlikely
Math is enticing
Could ya waste a paper, eg on energy?

Smaller ... larger

a thousandth of	Meters	
.001	milli	(0.0) kilo (1000)
.01	centi	mega (1E6)
a hundredth		

milli ... kilohertz
mega hertz

[redacted]

Aug 18 2015 (cont)

Three main factors that affect GC separation:

1. Boiling point, ie, or vapor pressure of the components
2. Carrier gas flow rate
3. Polarity of the column

You also understand columns much better now
Silica gel means that
Silica is the "support"
"gel" is the liquid, or equivalently, the
stationary phase.

You do not really know yet what the "gel" is
made of but you know that it is likely a
"liquid, wax, or low melting solid"
that is also non-volatile, has a high boiling
point, and a low vapor pressure

The liquid phase actually should dissolve
the components to be separated. That is why
a mid to non polar column does not work
especially well with water solutions.

Alcohol is probably fine to use when you
think about it.

Questions,

What, for example, could you dissolve in alcohol to test this out?

You know that the lipids dissolve in denatured alcohol but not isopropanol. This is a good example. But ~~Ethanol~~ is a denatured alcohol in a more complex mixture.
Try acetone, or xylene??

??? Question: Are the lipids actually volatile?
Heat them in an oven.

The materials to separate should dissolve in the liquid.

What happens if you use water @ a lower temperature? Does it just take longer?
How low in temp can you go?
Try 150 or 120°C next.

Aug 19 2015

Is Health 5 good or bad?

1. Have imported an excel file into a frame
2. Plots & Histograms
3. Summary Stats of the frame
4. Correlation between variables
5. Functions applied to variables.
6. Listing of objects
7. Get working directory
8. List working directory

Observations

1. 2 to 1 female
2. Health heavily skewed, 3 to 1 towards 4 & 5 vs 1 & 2
3. No Correlation between health and age
4. Avg Age ~ 54
5. Avg Health 3.4
6. n=61 Full data, Incomplete data N= 74
7. Age is broadly distributed, but peak @ 60-65
8. On Health ~ 29 > 4 (3.2 to 1 skew)
   ~ 9 < 2
9. On Gender 48/26 = 1.9 almost 2 to 1 ratio.

Aug 19 2015

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Aug 20 2015

We are looking @ a statistical set of tests applied to the Farmers Almanac.

The results expose numerous fallacies & weaknesses upon the casual interpretation of statistical tests.

The problem arose because of the contradiction of apparent success between the maps and the failure of temperature prediction. The maps look reasonably accurate. The temp predictions seemed to be flawed. But the temps are used to state an accuracy of 80% +.

Or temp data.
1. First, there is no correlation of significance between prediction & actual results
2. Secondly, there are zero values that appear to be used to sway the results
3. The data does not appear to be normally distributed at all, and yet the stat test used (z test) assumes that it is

Mean of prediction is -.62 σ = Ø.79
Mean of actual is -1.36 σ = 2.30

Mean of error is Ø.74 σ = 2.53

So what exactly does it mean when your dispersion on error is 3-4 the magnitude of what you are trying to predict?

Notice that neither the prediction or the error are normally distributed, they both have a significant negative bias.

But looking @ the data graphically, we can see that they did indeed get it right.

What is a box whisker? Got it, min, max, median, 25th, 75th
So the section Farmer Almanac has got it quite right.
Farmers Almanac actual

and the error are actually more closer to being more normally distributed than the prediction.

MRP
~~OFC~~ Column is a problem. [redacted]

Aug 20 2015

MRP - First results - Completed surveys - N=76

Age: Median 56.50
Mean 53.7
Max 76
Min 23
Qtrs 44-64

Health: 3.0
3.4
5
1
3-4

Gender: M 26
F 48
NA 2

Trend: Declining 41
Improving 10
Stable 24
= 34

Content:
Disappointed 37
Content or Very Content 37

Tobacco
Moderately or Regularly 24
None or Rarely 50

Alcohol
Moderate or Excessive 17
None Rarely 50

OTC/Supplements
Yes 56
No 18

Prescription
Yes 35
No 30

Rec Drugs
Yes 12
No 61

Exercise
Moderately or Regularly 50
None to Rarely 25

I am not so sure that it make any sense to try and 'analyze' the demographic data it serve primarily to identify the population of the survey.

But you can still ask questions. Is your sample representative of the general population? What exactly is the general population. What chance is that that the female / male ratio is unique?

eg Tread $n = 15$

$X_1 = 41$ $\quad P_X = 45.3$ %

$X_2 = 34$

$$z = \frac{[37.5 - 34] - .5}{(37.5 * .541)^{1/2}} = .66$$ Not even close to beg significant

Now male vs female

$X_1 = 26 \quad n = 14$

$X_2 = 40$

$$P_X = \frac{26}{74} = .35 \qquad z = \frac{|37 - 26| - .5}{(37 \cdot .65)^{1/2}} = 2.14$$

Significant @ the 96% level

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Significant @ the 96% level

My distribution

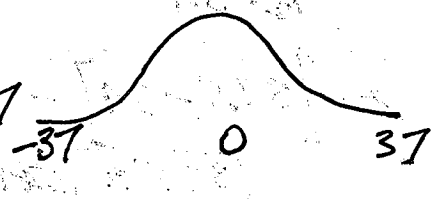
Decimal form $Pr = \left(\frac{200}{\pi}\right) \tan^{-1}(C \cdot x)$ / 100

$C = \frac{1}{Range} \cdot \tan\left(\left(\frac{RangePr \cdot \pi}{200}\right)\right)$

$Pr\% = \frac{200}{\pi} \tan^{-1}(C \cdot x)$ x is the value

Eg Assume Range Pr = ~~99.99~~ 100%

Range = ~~37~~ ~~74~~ 37



$C = \frac{1}{37} \tan\left(\left(\frac{100}{200} \cdot \pi\right)\right)$ = ~~3.70E-4~~ ~~7.4E-4~~ 7.411E-4

If we use 37, $Pr\% = \frac{~~49.93\%~~}{~~99.85\%~~}$ This is not really.

37: Pr = 99.993% Not bad

So if $x = 26$, $Pr = 70.3\%$

Which is not really that significant.

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mediterranean

The conclusion from your distribution is that

~~Is there a 70% Chance that women are more likely to fill out a questionnaire than men?~~

I would say yes, absolutely

Are women 1.4 times as likely to fill out a health questionnaire than men?

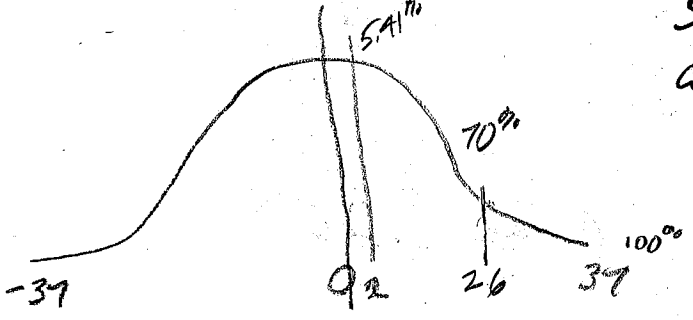
Quite conceivable.

I don't think that the bias is all that unusual

We get 1.85 to 1 vs theoretical 1.4 to 1.

Binomial Theorem says not significant @ the 96% level

I do not believe it



So 2 would be significant at the 100 - 5.41 = 94.6% level

but 26 is only significant at the 100 - 70% = 30% level

then not really significant.

What are national norms?

To compare to norms, you would ask

32% 1. How many people use tobacco regularly?
25% 2. How many people use alcohol?
76% 3. How many people use OTC & supplements?
48% 4. How many people use prescription drugs?
16% 5. How many people use recreational drugs?
67% 6. How many people exercise regularly?

Example, let's say n = 3000
& tobacco is @ 27%
and CA is n = 76
& tobacco use = 32%
are they different?

Non-Parametric

Aug 21 2005 n = 383 Chi Square Test for Independence

Poor Good

♀ 107 Health Rating 3.2 1-5

♂ 75 Health Pattern 2.3 Declining 1-3 Improving?

Health Content 2.4 Disagreeable 1-3 Very Content?

Skin Nails Ranking .5. Age → Overall Health .23 Chi Square

Demo Age Age → Health Pattern .20

Overall Health Rating Age → Skin Nails Ranky .6. .06 *

Age .5. .31

Age .7. .0006 *

Age .8. .02 *

Overall Health Rating ⟷ Skin 7 = .13

Health Pattern

Content Present Health

Skin 5-6 .01

~~5-7, 5-8 None~~

6-7 .06

6-8 .04

7-8

Age 191

Skin 5

6 80

7 72

8 63

Page 270

The χ^2 test in the Casio Classpad is fantastic.

i.e., does Age influence skin problems?
does grade level affect the grade received?
does anything 1 affect anything 2?
Categories of / Categories or classes
Classes

Educ. Level	Freshmen	Sophmore	Junins	Seniors
Grade				
A	25	12	25	18
B	41	31	50	20
C	78	57	25	12

from Casio χ^2 applied to a matrix entered
$p = 1.25E-6$ $(100\% - 1.25E-4)$
definitely not independent!

This is really cool.
Like Type of Cars
vs

			25 yrs	75 yrs
Low	Miles		6	16
Med	Per	eg	3	24
High	Gallon	# Miles	2	17

$p = .23$

95% Probability w/ Sets of data is not very strong.

So I generate some random numbers in a matrix

	Category 1	
	6	16
	3	24
	2	17
Category 2	4	21
	12	18
	42	3

and I get a P = ~~4.00E-13~~ 1.94E-13

What does this mean?

It says Category 1 influence Category 2?

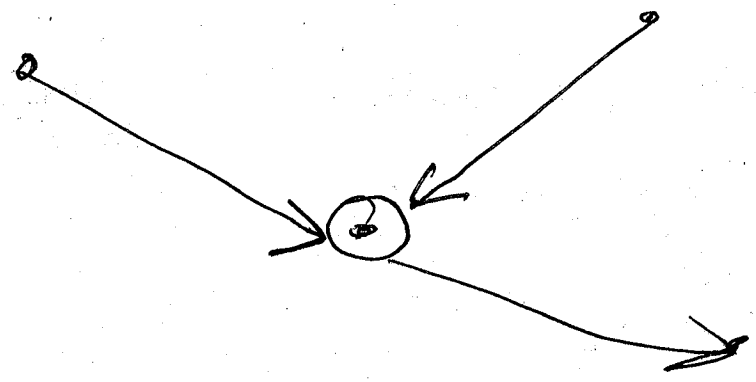
How is ~~the~~ possible?

The conclusion to be reached is that the two groups are not independent of one another.

How & why?

5. What does χ^2 actually mean?

Well a linear regression actually comes out strong also. The 42-3 set is skewing the data strongly.



Dems	Age
33	48
68	54
40	38
62	48
61	73
39	
62	
39	
64	
58	
44	
34	
46	
57	
61	
58	
56	
62	
57	
50	
57	
41	
32	
29	
56	
63	
62	
54	
23	
55	

I do not know how to make sense of the plot of age against them.

I do not see any pattern in the data.

Not true. You plotted the wrong set

Age - Stm 7

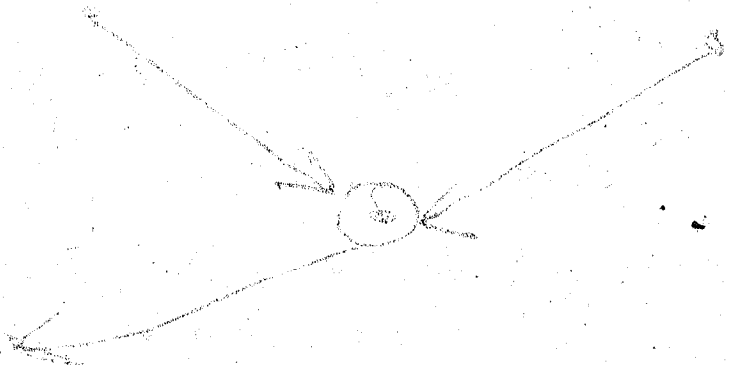
Shows a cluster in the data w/ a maximum set of value near the mean age.

Between Stm 5-6

There is also a cluster

Regardless of what 5 is, 6 is high.

But especially when 5 is high then 6 is high.



Health Rating & Health Pattern $p = 2.71E-9$
Health Rating & Content w/ Present Health 2.2E-16

Overall Health & Contentment of Health are ranked opposite of one another.

Health Rating: 5 means ~~stable~~ good Health. (poor health = 1 — good health = 5)

~~Contentment: 1 means very Content.~~

Contentment: 3 Disappointed, 1 very content

So they are inverse of one another.

Health Pattern Trend: Stable 1, Improving 3, Declining 2

Ok, we have done our first ANOVA (one way problem) w/ Casio and we know how to interpret Casio.

Now think about how to apply this.

One independent & on dependent variable.

Independent could be age. (is this really independent)

No. 1 How to apply in the problem.

Simulated MRP Anova

Continuing to develop application

	# Skin Conditions	# Skeletal Conditions	# Neural Problems
Subject 1	5	2	7
Subject 2	3	8	5
Subject 3	2	3	4
Subject 4	4	2	2
Subject 5	6	1	4

temp eliminate

adjusted

temp eliminate

$P = .67$

Conclusion means are not different

$P = .039$ with adjusted set

So now we know that there is a difference between the means of the groups. What is the difference & how does it lie?

Also, what if we were missing data?

Need completed surveys 3 sets of data.

We learn that Casio will handle unequal sample sizes. That is great.

Temp Elimination: $p = 8.2E-3$

$= .008$

w/ eliminated data.

You can also work w/ 2 columns & unequal sample sizes. That is good.

This is great. It means you now can have unequal sample sizes (Independent Variables)

Subject	# Skin Conditions	# Skeletal Conditions	# Neural Problems
1	X_1	X_1	X_1
2	X_2	X_2	X_2
3	X_3	X_3	
4		X_4	
5		X_5	

You can solve this

Lets see if we can get the two way ANOVA to work in Casio

We have learned how to input a 2x2 Multi ANOVA into Casio using the list editor.

Enter in spreadsheet just like this in two rows

113	139	133	126
116	132	131	122

means this

Ok, we now have it in the spreadsheet form accurately. So the actual structure of the data is:

	B	
A	113 116	139 132
	133 131	126 122

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Two Way Anova
Excellent Example

I have succeeded w/ an example problem from Statistics Explained by Hinton (Green-Balloon cover) on p 176.

This is interesting. Even though there are lots of measurements in each group it is still a 2×2 matrix

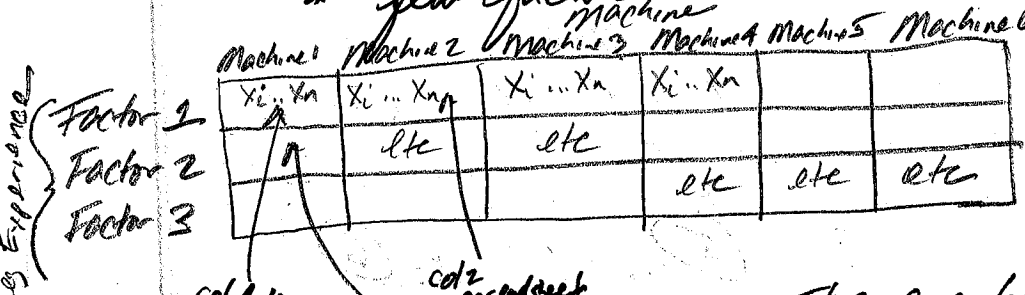
We are measuring the number of errors made by a worker with a particular machine.

Experience (A)

	Machine: B_1 OLD	Machine (B): B_2 NEW
Novice A_1	4, 5, 7, 6, 8, 5 — enter as Column 1 in Casio Spreadsheet	enter as Column 2 in Casio Spreadsheet — 5, 6, 5, 6, 5, 6
Experienced A_2	1, 2, 2, 3, 2, 3 — Enter as Column 3 in Casio Spreadsheet	Enter as Column 4 in Casio Spreadsheet — 8, 9, 8, 8, 7, 9

It is still a 2×2 no matter how many measurements in each box. I know that you can have only 2 measurements in a box (maybe you can even have only one?)

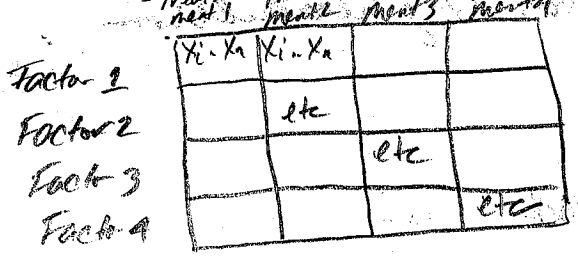
You see now that Cano can actualy handle up to a 3×6 and even a 4×4 so that is quite a few factors



This is a lot of data to handle.

Facto 1 = Novice
Facto 2 = Journeyman
Facto 3 = Master Craftsman

You could also have up to a 4×4



This is a lot of data to handle

Now, our Cano results are $A_p = 0.21$
$B_p = 4.5E-7$
(This is not just the straight product $AB_p = 8.3E-8$ of $A_p \cdot B_p$ No!
Now, how to interpret results: (From Hinton)
the answers of

A_p 1. Experience on an old machine is not significant.
B_p 2. The effect of the type of machine is very significant
AB_p 3. The interaction of experience & machine is also highly significant.

Two way Anova is really an interesting situation.

Two way anova is really interesting.
What if we only had 1 data point?
Can we still solve it.

	(B1) OLD	Machine Facto B	(B2) NEW
Novice (A1)	4 5 7		5 6
Experienced A(2)	1 2		8 9

Experience Facto A

Can this be solved?
It does not look good. It generates Errors.

Now try (2 nos.)

Yes 2 numbers Work

Ap = .9999 (no effect)
Bp = 1.33E-3 (significant)
ABp = 3.9E-3

So only two data points for each situation still picked up the results strongly.
This is really amazing.

Can it work with uneven data?
Yes it can

This is very valuable

Now let's look how to apply this. (Uneven data sets allowed)

Body Flags is a Factor

We have systems of the body.

	Total Flags Skin	Total Flags Neural	Total Flags Vision
Young	$x_1 \dots x_n$	etc	
Middle	$x_1 \dots x_n$		
Elderly	$x_1 \dots x_n$		etc

Age is a Factor

This alone is a 3 x 3 ANOVA

Smoker

Yes			
No			

This is a 2 x 3 ANOVA

Health
- Poor
- Stable
- Good

3 x 3

Sex
- Male
- Female

We have 3 Health Factors:
- Health Rate
- Health Trend
- Health Contentment

Overall Health = Σ

MRP Questions:

Now, what you are thinking about, is,
What do you really want to know?

1. Is there a segment of the population that is reporting the same Chronic health symptoms?

2. If so, what type of health symptoms are they reporting?

2b. What type of profile is reporting these symptoms? (eg age)

3. How many people are reporting these health symptoms?

4. If so, have they been diagnosed & treated?

5. How effective have the treatments been?

6. Is there a relationship a correlation between the type of symptom that are being reported? (eg skin vs neural)

7. Are there any patterns of exercise drugs, alcohol, etc that accompany the reports.

8. Is there any distribution of the symptoms or demographics in general?

I am confused on Casio,

Casio only allows for the solving of a 2 way anova problem.

This corresponds to a 2×2 matrix

		(B_1)	B (B_2)
A	(A_1)	$X_i \cdot X_n$	$X_i : X_n$
	(A_2)	$X_i \cdot X_n$	$X_i .. X_n$

So why does Casio allow an input table up to 4×4? I do not understand this @ all.

They do not allow for the solution of a 2×3 for example, but they seem to provide a data entry format for it, I do not understand this

Hinton has our answer p186
There are at least 3 variations on the 2 way anova, & even though a 2×3 matrix might be involved, it is still a 2 way Anova! You had good notes in that book that explain the situation. You have to think about what actually are factors vs categories or classifications of the same factor. Factor 2 (Time)

Factor 1 (Experience)	1 week	2 week	3 weeks
Novice			
Experienced			

Even though this is a 2×3 matrix It is still a 2 Way Anova!

Ok, I have figured the example of Hinton p 181 - 192
and Casio has it right.

It is a 2x3 matrix BUT IT IS STILL A 2 WAY ANOVA!

Let's interpret the results starts on p 190. This is going to be interesting.

So you can have only two factors but you can have many subdivisions of that same factor.

Health Conditions
Skin Blood Vision Neural etc
these are all variations of a health condition

Overall Health Factor

Poor
Stable
Good
Improving

	Hair
1	4
2	5
3	6
4	5
5	6
6	4.5
7	5
8	3.5
9	4
~~X=3.5~~	
~~σ=1.1~~	
X=4.9	
σ=0.88	

Aug 23 2015 n=86 Completed Surveys

$\bar{X}$ 53.3 Age

M 31 F 52 MRP Survey is already revealing very interesting data

Gender Male Female

$\bar{X}$=3.4 Health 1= poor 5= excellent

$\bar{X}$=2.1 Pattern Stable 1 Improving 2 declining 3

$\bar{X}$=2.4 Content Very Content 1 Somewhat Content 2 Disappointed 3

$\bar{X}$=1.9 Tobacco none 49 rarely 5 moderately 16 regularly 13 excessively

$\bar{X}$=2.1 Alcohol none 22 rarely 34 moderately 18 reg. 6 excess. 2

$\bar{X}$=1.3 OTC/Sup Yes 61 No 22

$\bar{X}$=1.5 Prescription Yes 37 No 44

$\bar{X}$=1.8 Rec Drugs Yes 17 No 65

$\bar{X}$=2.9 Exercise None 2 Rarely 20 Moderately 36 Regularly 20 Heavy

Skin & Nails 1-16

			Eyes	
5	1	Materials emerging	1	3
6	2	Materials seen or felt beneath surface	2	4
9	3	Lesions	3	3
9	4	Pimples/acne	4	4
10.5	5	Rashes or other skin conditions	5	3.5
12.5	6	Unusual appearance or changes in skin texture	6	5
11.0	7	Loss or increase of skin pigmentation	7	5.5
10	8	Observations of pigment or fluorescence		Y N
9	9	Sweating	Diagnosis	16 67
8.5	10	Coatings or films	Treat	15 67
6	11	Unusual fingernails or toenails		
7.5	12	Ingrown hair	~~$\bar{X}$=4.0~~	
6	13	Changes in body hair	~~σ=0.9~~	
5.5	14	Motion under skin	$\bar{X}$=4.0	
6.5	15	Motion of extraneous item	σ=0.96	
12	16	Painful or irritating sensations on the skin		

$\bar{X}$=8.4

σ=2.4

	Yes	No
Diagnosis of Skin Conditions	24	62
Treatment	30	52

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n = ? 86

Now, isn't this a perfect One Way Anova Problem?

Yes it is. Fact = Health Factors

	Skin	Hair	Eyes
measurements	X_1	X_2	X_3
	⋮	⋮	⋮

99.9999% (Skin) Hair Nails: Anova: $A_p = 5.96E-6$ $p < .01$

~~99.9999%~~ 80% Hair - Eyes Not Significant $A_p = 0.11$ $p > .05$

99.95% (Skin) - Eyes $A_p = 4.7E-4$ $p < .01$

99.95% (Skin) - Hair $A_p = 4.51E-4$ $p < .01$

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Skin is highly significant.

Error MS (variance) = 3.312

$df_{error} = 29$ $p = .01$

No. of Conditions $k = 3$ $Q = 4.45$

$4.45\left(\frac{3.312}{\#\ \text{of reps}}\right)^{1/2} =$ ~~2.04~~ 3.09

If picked a larger p

p 142 Hinton formula leads to n = 9.5 which makes results even better.

if a difference in means is greater than 2.04 then it is significant

Significant 99% ~~Significant 99%~~ Not Significant @ 99%

~~8.4~~ 8.4 - 4.8 = 3.6 which is > ~~2.04~~ 3.09 Skin vs Eyes

8.4 - ~~3.6~~ 4.0 = ~~4.8~~ 4.4 which is > ~~2.04~~ 3.09 Skin vs Hair

4.8 - ~~3.6~~ 4.0 = ~~1.2~~ 0.8 which is < ~~2.04~~ 3.09 Hair vs Eyes.

The average profile.

1. 53 years old
2. 63% Chance of being female
3. Health slightly above average
4. Health is slightly declining
5. Somewhat disappointed in recent health trends
6. Rarely uses tobacco
7. Rarely uses alcohol
8. 73% Chance of taking OTC or supplements
9. 46% Chance of taking prescription drugs
10. 21% Chance of taking recreational drugs
11. Moderately exercises

Two things to do:

1. Learn the third variation of a 2 way anova
2. Learn how anova is used in R
   You are using a 2 way anova only so far
3. Could you set up your one way anova as a 2 way? 2 way needs a minimum of a 2x2 matrix so no you cannot
4. What is a test for means?
5. Need a test for normal distribution.

We have got another variation on the 2 way Anova:

Subject measurement	Factor 1		Factor 2	
	Factor 1A	Factor 1B	Factor 2A	Factor 2B
1	X_i	X_i	X_i	X_i
2	⋮	⋮	⋮	⋮
3				
⋮	X_n	X_n	X_n	X_n
n				

Is this a 1×4 matrix?
a 4×1 matrix

I cannot set this from table of in Casio however

Can we add a notes column? Can we have a 1C? Can we have a 2C? Can we have a 1C but not a 2C?

We now have 3 variations a 2 way ANOVAS

Factor A

	B_1	B_2
A_1	OK	
A_2	Casio	

	B_1	B_2	B_3
A_1	OK		
A_2	Casio		

	A		B	
	A_1	A_2	B_1	B_2
1	X_i	X_i	X_i	X_i
2	⋮	⋮	⋮	⋮
3	X_n	X_n	X_n	X_n
⋮				
n				

Not OK in Casio so far

They are each 2 way ANOVAS.

There are some great accomplishments of Casio on these. There also appear to be a lemon on the format of 2 way ANOVAs but it can accept 2 out of three presented by Hinton.

One way anova are very easy in Casio.
Anova also allows for unequal sample sizes, even in Casio, so this is great.

What are the assumptions of ANOVA?

How do you tell if data is normally distributed or not?

Looking @ all data n = 397 394

Skin	~~Avg of medians is~~	Hair		Eyes	
1	5	1	3	1	3
2	6	2	4	2	4
3	7.5	3	5	3	3
4	9	4	5	4	5
5	11	5	6	5	3
6	13	6	5	6	5
7	12	7	5	7	3
8	11	8	5		
9	9	9	3.5		
10	10				
11	7				
12	6.5				
13	6				
14	7				
15	8				
16	9				
$\bar{X}$ = 8.6	σ = 2.34	$\bar{X}$ = 4.6	σ = 0.93	$\bar{X}$ = 3.7	σ = 0.95

Skin, Hair, Nails
Err MS (variance) A_p = 8.30E-7
Err df = 3.27
= 29

Skin - Hair A_p = 7.44E-5
Hair - Eyes A_p = 0.08
Skin - Eyes A_p = 3.49E-5

Tukey Test : .01 = p

$q = 4.47$ (Hinton p=.01 p 366 interpolated)

$HSD = 4.47\left(\frac{3.27}{7}\right)^{1/2} = 3.06$

	4.6	4.0		.01
Skin - Hair :	8.6 - ~~3.06~~	= ~~5.54~~	> 3.06	Significant
Skin - Eyes	8.6 - 3.7	= 4.9	> 3.06	Significant
Eyes - Hair	4.6 - 3.7	= .9	< 3.06	Not Significant

? Skin - Hair Nails Anova Ap= 8.30E-7

T Distribution explination:

x = 4 df = 29 p= 5.43E-4 .00054 *100= .05

x = 5 3.52E-5

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Aug 25 2015 Back in Wallace

GC Testing.
Xylene is highly polar so the clots not work.
The lipids are highly polar so they do not work.

Alcohols have a lot of water in them so they may not work.

What is a person to do?

Compare Acetone
Isopronal
Denatured alcohol?
How do you use the instruments then?
What do you put in it and how?

1. Check sample w/ oven first?!
2. Blood and capillary tube

Aug 27 2015

Tonight we learn something about solvents & their suitability for GC.

Alcohol has their problems; especially if they have any water in them.

Acetone also has it problems as it is highly volatile & flammable as well so it has some hazards. It also did not dissolve any organics from tea so it is not at all the same as an alcohol.

MEK ends up being a very interesting solvent. It is miscible w/ water and does not centrifuge out so it is partially polar. It has the formula C_4H_8O so it is still a lower hydrocarbon. It has a boiling point of 80°C (175°F) so it is much safer to work with. Now, does it dissolve tea?
So far, very mildly, but better than acetone, not nearly as well as alcohol.

MEK @ 100°C gives a nice peak @ 0.610 ~ 3mV. Am using high current. I do not anticipate a water peak as in alcohol.
With mild tea extract I will run a program for 6 10 min @ 100, ramp @ 10°/min to 180° and then hold @ 180 for 10 min.

Late we will shift to low current.

You are correct that MEK looks to be a very good solvent to use, assuming that you can dissolve organics (& fibers) within it.

Indeed it does not look like you are going to have the problem of detection that alcohol does, especially those w/ water as them.

You also see that you only want to have temps @ 10° per min, not 20°C & it will hold the baseline better.

W/ our tea and MEK, something seems to be happening @ 130–160°C. It could be the temperature ramp characteristics.

Levels off @ 5.8 mV @ 19 min while ramped from 100° to 180°.

The problem is that it does not seem to be detecting anything.

Perfectly flat after ramp stabilization.

Next program (no additional injection) is from 180 (2 min, ramp @ 10°C) to 230°C.

Detector now @ 240°C

Max Oven Temp = 210°C

I do not know why?

Something happened @ ~220°C.

It triggered circuit alarm again.

I think we need to try keeping the current set on low for now.

Lets try the run again under low current.

Something happen @ 220°C ???

Trigger circuit again.

Try: Detector @ 200°C setpoint (30° above)

also set ramp @ 5°C, not 10°C

Something trigger @ 222°C

Lesson do not go above ~~220°C~~ 210°C

I do not know why

But this should be sufficient.

The headers look clean @ 210°C 6 min.

MEK still looks better to me.

Ask about 220° limit on Facelook.

I see no indication of any residual in the column @ 210°C @ 15 min. Assume it is clean.

45 - 60 - 150 MEK Tea:

There is a good MEK peak @ ~ Ø.6 mV, the baseline is. There appears to be no water contamination, which is also fine. But and a big but it is, you see no additional tea peak yet up to & including 210°C. ???

Notice the MEK peak is quite small, about Ø.1 mV. We can try next run with higher currents. The shower, run @ 45°C. So it did not need much to leave the column.

We apparently did not dissolve very much? Stronger solution?

Aug 27 2015

Time to start digging into a Cal analysis (tea)

1. We know that MEK seems like a very good solvent to use w/ no distortions.

2. We see that tea dissolves (extracts) very well into ethanol but not well at all compared to MEK.

3. The idea, therefore, is to extract the tea into ethanol, and then take a small portion of that into predominantly MEK.

4. We are querying 2 small peaks that are showing up with a 45°-60° ramp.

0.28 mV	question
0.65 mV	MEK (possibly the ethanol also)
7.82 mV	something very small happened.

5. Let's go back to control w/ MEK w/ 45-60 (control w/ pure MEK shows the same small peaks @ 0.28 so it may be nothing.

What you all have is that there are 4 small peaks that precede the solvent peak.!! What is all of this activity?

No small peak showed up @ 7.82 min. We may have something there.

Even 40°C on the column is still 100°F.
60°C is 140°F
These are actually reasonably high.

Ideas:

1. Dissolve the organics in any miscible solvent w/ MEK that works. Make as concentrated as possible.

2. Add concentrate to MEK or primary solvent. Minimize alcohol & water content.

3. Consider very low temperatures (frost & study them thoroughly, even over extended time.

4. Bake out water & alcohols when you are done.

MEK Control: We actually have peak @:
0.12 m .136 mv
0.19 m .049
0.27 m .043
0.61 m .919

If you can repeat the peak @ 7.82 We will switch to hyd carrots

There is no peak @ 7.82 min w/ the MEK tec that is that is not reproducible yet.

But what provides the solvent peak is getting to be interesting. We have peaks @

0.10 m , 296 mV
0.23 m , 071 mV
0.29 m , 028 mV
0.65 m , 648 mV

What we see, therefore, is that these peaks are repeatable, even from w/in the MEK control.

This strongly suggests that we have some more polar "contaminants" in additive, or? in the MEK that are eluting very early.

We do not pick up any known tea peaks.
Let input the alcohol version to see how it behaves and drop temperature down to 40°C.

Ok, we have input the MEK tea in under high current condition @ 40°C.
We have very high sensitivity here!

We are learning that what is happening w/in the first minute is a LOT and that it potentially is very important.
We should look @ N_2O_2 peak.

to when we are dealing w/ small peaks, & maybe even lower temperatures, also in where the high current setting can make a big difference.

You have been using the instrument handbook that you need to.

	Peak @	
filtered & smoothed	Ø.11 m	.330 mV
	Ø.35 m	.067 mV different
	Ø.67 m	2.969 mV

2-3 times as sensitive w/ high current.

Remember that we lowered temp to 40°C. This can change relative trans.

DO NOT SMOOTH THE DATA w/ small peaks.

Peak @	
Ø.10 m	.440 mV
Ø.18 m	.156 mV
Ø.21 m	.162 mV
0.66 m	1.139

Peaks: MEK w/ tea

~ .08	first peak	Repeatable
~ .11	.348mV	
~ .19	.067mV	
~ .23	.10mV	
~ .67	1.558mV	

Now let's fly to the alcohol based extract. Use 40-60. Hold On

Hold on! Do air first & learn about N_2O_2 @ 40-60 Air first

Ok, this is very interesting. Peaks @

.05m 5.905
Ø.52m 2472 mV !!! What is this?

The Solid Calibration Chart also shows the initial peak. What is it?
Notice that are not the same as with the solvent except for .08 has the same negative reversal.
Could it be hydrogen? What is it.
Now extend to 10m @ 40°C

The CO_2 peak was easily picked up. Very sound @ 40°C.
Lower temperatures are not sensitive.

.05m	6.09mV	
.39m	.082mV	?
Ø.5	2607mV	O_2 N_2
6.59	.324 mV	CO_2
? 8.88	.014	

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There is more Sorry on in the atmosphere than needs the legs also.

Sample 2

There are reproducible peaks

		left	right	top magnitude	bottom mag
Unknown 1 ? 176ppm	.05 m	.04	.09	5.837	-.09
Unknown 2 ? Ø.4ppm	.40	.38	.41	.142	.120
O_2N_2 99.91%	.52	.43	1.13	.2410	.293
CO_2 157ppm	6.57	5.87	7.37	.265	.089

8.88 is uncertain What

Sample 1:

Unknown 1 180ppm	.04 .05	.04	.09	5.906	0
Unknown 2 Ø.4ppm	.40	.38	.41	.143	.119
N_2O_2 99.96%	.52	.43	1.11	.2412	.269
CO_2 111ppm	6.56	5.91	7.51	.268	.079

8.86 is a candidate.

What are the 2 unknowns?
What was the one that is so high?
What is methane?

Helium	.143
CO_2	.015
O_2	.024
N_2	.024
Argon	.016
Methane	.03

Composition of Air

$O_2 + N_2 = 78.09 + 20.95 = \underline{99.04}$

Argon	1.0%	10,000 ppm
CO_2	.0345%	345 ppm
Methane	.00017%	1.7 ppm
Nitrous Oxide		.305 ppm

This suggests that you are indeed detecting methane.
Two big questions.
1. Why do you not detect argon since there is 30 times more than CO_2 in it?

2. What is the unknown situation with respect to Peak 1 since it is of the same magnitude as CO_2

Our Questions?

Source say that argon is very difficult to separate from O_2.

I believe we have methane which I don't think anyone would believe.

Then a really getting interesting.

What you are really measuring is O_2 N_2 and Argon together.

We get: $\frac{(99.967 + 99.964)}{2} = 99.965\%$

This should include O_2, N_2 & O_2 from a space:

$O_2 = 21.0\%$ $\quad CO_2 = .0345\% = 345 ppm$

$N_2 = 78.0$ $\quad$ methane $= .0017\% = 2 ppm$

Ars $= 1\%$

$\sim 100\%$

But we have a remainder of $.034\% =$

1% of a million $= 10{,}000 \sim 10{,}000 ppm$.

$.034\% = .00034 \left(\frac{10{,}000}{10{,}000}\right) =$

Let's run a trivial recovery the first unknown peak.

This leads to 99.982% O_2 N_2 O_2

with a deficit of .018% = 180 ppm

We measure CO_2 @ $\frac{(156+177)}{2}$ = 166 PPM

We measure Methane @ 0.4 PPM

So if we scale our trace gases to 180ppm we get

~~179 PPM CO_2~~ This shows both CO_2 & Methane reduced.

Current data shows ~~400~~ 401 ppm

This scales out to be

(166 → 401) (ratio is 401/166) = 2.42

So

2.42(0.4) = 0.97 = 1 PPM Methane

Alcohol Tea run.

Some interesting things seen on the run @ 40-60 degrees showed nothing.
We are baking out now @ 180° for 30 min.
The "water" peak shown up exactly as anticipated, it is always a major feature.

You are on a dry run w/ the residual.

0.9 minutes. - Maybe something.
3.5 m] two small peaks show up.
3.8 m] here, that appear new.
12 m. The major water, alcohol peak.

These are in addition to 14 min @ 40-60 deg.
Therefore lets assume we go @ 120°

$\frac{50^\circ}{120}$ = this reduces 1st set to 6 min

Now take 4 min @ 120 $\frac{120}{100} = 1.2\ (4\text{ min}) = 5$ min

6 + 5 = 11 13
Therefore we will run 15 min @ 100 w/ alcohol tea.

Conditions of run will be

1. Alcohol Tea
2. 100°C – Isothermal
3. High current setting
4. 13 min.

Alcohol is described a tough but as far as it is the only way that we can dissolve (i.e, extract) the tea.

Alcohol really don't look problematic to me.

You are producing a lot of peak very likely out to 20 to 30 min as well as Carrier Delta Cake. We are all on the way now.
There seems to be a whole lot going on & then in after the water peak.

There appears to be a lot of contaminants in the Column & Septa in a very complicated mixture.

It looks like some very serious cleaning took place here. The tea may be far too complicated to be looking @?

The late night trial Concentrate ~~MEK~~ + Ethanol flea & mixed roughly 50-50 w/ MEK. Run is @ 100°C isothermal for 30 min w/ high current. No signs yet of mixture.

We are barely the baseline only 10 minutes.

It is possible that we have some very minor activity @

3.26 m very weak ?
21.91 m very weak ? } uncertain

We will have dry run @ 150°C for 15 min.

The good news is that we still do not see a weak peak. (@ 30 min 100°C + 7 min 150°C)

No activity seen.

Now @ 200°C for 15 min

We have a very broad wide stray tally peak that started @ ~ 6 min, reached @ ~ 8.6 min and then trailed gradually. Wait again? 30 mV.

Not done. Rerun dry tomorrow @ 200°C 210°C extended

Denatured alcohol alone might produce this Title #35 Aug 28.

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Denatured alcohol alone might produce this Title #35 Aug 28.

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Aug 26 2015

We see clearly now that we need a non-polar column.
This means that polar compounds (water & alcohols) will pass through the column quickly, giving discernible peaks.

The is opposed to what we have, which is clearly a Polar column, which means that non-polar compounds, such as solvents, pass through quickly & give very discernible peaks.

We wish to explore polar compounds (water, alcohols) as quickly as possible.

Lets compare Naptha by itself, MEK by itself & Naptha MEK mix.

all have to be done @ 45° to be able to compare them

You can also see now that you had some contaminents in your earlier MEK runs (small peaks).

MEK
Naptha MIX is @ 0.66 .867
Naptha alone is @ 0.65 .675mV .864

You cannot tell them apart @ all.

SR1 sells SS is Stainless Steel

Hayes sep D 290° (250)

Hayes sep N 165° Does not look to best either

ParaPack Q

They say they separate Love T also.
Highest polarity
does not look to best

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Guess what?

Just because something dissolves does not mean that it is volatile.

Salt dissolves, but it is not volatile.

It dries up as a crystal and would plug everything up & cause damage to the equipment.

Flushing w/ water may indeed be a viable approach to cleanup.

Conclusion on Naptha Tea & MEK Tea Runs

Naptha Tea & MEK Tea show no detectable components at this time.

You can run a Naptha control again to verify this.

The idea did not work so far.

Alcohol extraction gives you problems
We need the new column.

We have an interesting observation.

The "lipids" behave like any other solvent in the GC.

This could be disconcerting.
What is the refractive index of xylene?
It is 1.478 vs 1.492 so they are not the same.
Nevertheless, I think that your hunch is correct, the CBB "lipids" could well be lipids that have dissolved w/ in xylene". An interesting proposition.

Now, the next topic. We last charged gases.
We see that we have a polar column. It therefore detects non-polar well (at least earlier in the process). We also learn that all solvents behave essentially the same because they have very similar thermal conductivity values.

We therefore see that the most likely early and easy detects will be the dissolving of "other" non polar substances, such as essential oils, camphor etc at the trace levels w/ in the non polar solvent. This should allow Ga to detect "other" hydrocarbons / or non polar compounds to varying degree

As such, we are now experimenting w/ 1 or 2 drops of camphor phenique w/ in approx 1 ml of naptha. We may have some results. We need to use light current.

I am baffled. I see nothing @ 45°C except for solvent.

SUCCESS has been ACHIEVED.

The entire process was predicted before it occurred. It is a marvelous experience.

Method

1. Solvent is Naptha (approx 1 ml) } Both
2. "Contaminant" is Campho Phenique } Non Pola
3. Temp is 250 Isothermal for 20 min
4. Last peak ends @ 13 min.
5. Very clean separation.
6. Miniscule solvent peak @ front of Chromatogram.

When a Polar Column

You should be able to detect @ fraction much much lower than this; the peaks are huge & broad, but also well formed.

7. Naptha was a perfect choice for a solvent. No water dissolution.

8. Baking at and leaving temp over 250 & detector to 280 appears to have been critical to success. The Columns now appear very clean.

You have therefore learned, as well a predicted, that your GC column is currently configured for non-polar detection of "Contaminants" or Components w/a a non-polar solvent that use a polar Column.

So now a question: Can you dissolve tea in a separate non-polar substance such as mineral oil?

You need to extract into a polar solution but not the solvent.

Next: 10ml Camplo Phenique
1 ml Naptha
Low Current
250°C isothermal

You are getting amazing results. You have picked up even another peak now (small).

You may be picking up mineral oil & Eucalyptus oil as primary peaks? Who is the small peak?

So try mineral oil next.

Aug 29 2015

Tennant is saying voltage = pH

I determine relationship as

$y = -.0172x + 6.988 \quad r^2 = .9995$

where x is voltage so

$pH = -.0172 \cdot Voltage + 6.988$

or

$Voltage = -58.22 * pH + 406.07$

The signs on my meter are reversed from what Tennant says

Is this the same as oxidation potential?

~~It our meter seems to have reversed the signs.~~

This leads to models:

~~Wrong~~

$Voltage = 58.22 * pH - 406.07$

$pH = .0172 * Voltage + 6.99$

or more practically.

$Voltage \approx 58.2 * pH - 407.0$

My Meter

$pH \approx .0172 * Voltage + 7.0$

mV	pH
506	5.0
555	2.7

The more positive the potential the greater the species affinity for electrons. ORP is a common measurement for water quality

It is measuring its potential as an oxidizer.

So the lower the pH, the greater the oxidation potential. The greater the oxidation potential the greater the species capability to act as an oxidizer.

So now so back to the definition of an acid & a base.

1. An acid is H^+
2. An acid is an electron acceptor - it wants to gain (Second formula). "steal electrons, i.e. act as an oxidizing agent)
3. An acid is a proton donor.

Tennant Study

Neutral water is D. H$_2$O

Water range from −12 to 25

I measured +10 mV with my meter

A positive number means that it has oxidizing capabilities. (i.e. it wishes to combine w/ oxygen and steal electrons)

Negative means that it has reducing capabilities

Chlorination cause ORP in the range of 650 mV.!

Bacteria survive >300s when ORP < 485

< 30s when ORP > 665

Tennant		cell		Saliva
−20 mV	⇔	7.35	⇔	6.55 pH
−50 mV	⇔	7.88	⇔	7.08 pH