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Authored
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TOP GRADE

Chemistry Vol VIII

120

3 Subject

Perforated Sheets

• 10-1/2 x 8" • 26.7 x 20.3 cm

NOTEBOOK

College Ruled

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Lab Notes

Jan 2015

California! Jan 22 2015

We are looking @ a recursive converging series.
This is really interesting.
The series is:

n = 500
$a_n = .656$
$a_{n+1} = .6769$

$$a_{n+1} = -3a_n^2 + 3a_n$$

n=1 to 500
$a_1 = .01$
$a_n Str = .01$

There is a 2nd series of
$b_{n+1} = 3b_n - 0.2$
but it is not converging.

a_n Str is only for the graph
What does a series like this mean?
Why does it Converge?
Does it actually represent a difference equation?
eg
~~$X_{n+1} = X_{n+2} \Rightarrow$~~
$X_{n+1} = X_n + 2 \Rightarrow \quad X_{n+1} - X_n = 2$
This means the difference Δ is a Constant.
This certainly implies the function is a line
There should always be a function.
How do you know what it will Converge to?
In our web graph mode, we are headed towards $x=y$
yes, the b_{n+1} series has no significance here.

Convergence here means that $a_{n+1} \Rightarrow a_n$ approaches
Notice the series has no meaning if $a_n = 0$. So it has to start somewhere.

The plot in time also shows Convergence easily.

The starting pt affects convergence

It converges with $a_0 = .01$ & $a_0 = .5$ with no problem.
Not w/ $a_0 = \underline{1}$. $a_0 = .9$ IS OK

Now, insted of $a_{n+1} = a_n + C$
use
$a_{n+1} = Ka_n + C$

$a_{n+1} - Ka_n = C$

$f(x_{n+1}) - K(f(x)) = C$ This changes everything

This does not seem so easy to separate:
But this is a line, as essentially $\Delta f(x) = c$

Here is the case

$x_{n+1} = a x_n$ this is almost our case
$x_n = a^n x_0$ OK

n   If $x_0 = 1, a = 2$
1   eg $2 = 2 \cdot 1$ $x_1 = x_n = a$
2   $4 = 2 \cdot 2$ $x_2 = 2^2 \cdot 1$
3   $8 = 2 \cdot 4$ $x_3 = 2^3 \cdot 1$
4   $16 = 2 \cdot 8$ $x_4 = 2^4 \cdot 1$ etc

let $X = X(t_n)$ t = time

and $t_{n+1} = t_n + h$ $t_0 = 0$ $t_n = n \cdot h$

Rewrite

$X_{n+1} = aX_n$ as

where does this come from?

~~$X(t_n+h) x(t_n)$~~

ok look @ this. $\frac{X(t_n+h) - X(t_n)}{h} = \frac{(a-1)}{h} X(t_n)$ Check how to do this

Next we assume h is small, can be approximated by the differential equation

$$X'(t) = \frac{a-1}{h} x(t)$$

this has the solution

$$X(t) = X_0 e^{\left(\frac{a-1}{h}\right) \cdot t}$$

you know this.

$u' = ky$

So there is a relationship but it is not obvious.

Sure enough, the solution does have this form.

This is very interesting

$a_{n+1} = a_n + 1$ is linear

$a_{n+1} = 2a_n + 2$ is exponential

So a very big difference

If $k > 1$, it leads to an exponential form

If $k = 1$ " " " a linear form.

If $k < 1$ it converges toward an eventual value, it looks logarithmic

Three different coefficients, 3 different behaviors!!

I don't know how you would ever know that.

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Back to:

$f(x_{n+1}) - k(f(x)) = C$

How would you go about solving this?

$f(x+h) - k(f(x)) = C$

$\frac{f(x+h) - k(f(x))}{h} = \frac{C}{h}$

NO
T IS NOT ~~this is like $\frac{dy}{dx} = \frac{C}{h}$~~ or $\frac{dy}{dx} = \frac{C}{\Delta x}$

~~$y' = \frac{C}{dx}$~~

$= \frac{f(x+h)}{h} - k\left(\frac{f(x)}{h}\right) = \frac{C}{h}$

this is like $y(x+h) - k(y(x)) = C$

and if you graphed this: ?
or $y(x+h) = k(y(x)) + C$

The coefficient C also effects this a lot

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this is the answer to your question

so actually $x_n = x(t_n)$

What is Δh in a recursion equation?
Is it 1? How do we know what it is?
Well it is implicit in the recursion.
To relate it to a differential equation
h must become small.

So when we have
$a_{n+1} = ka_n + c$ we would like to look at
$f(x_{n+1}) = k(f(x)) + c$ in the form of
it is very interesting what we do.
we start actually with the form:
$x_{n+1} = ax_n$ where x is actually the functional result.
then we regard x as being
a function of time (but discrete time) so
$x = x(t_n)$
and $t_{n+1} = t_n + h$] this is the shift in thinking.

!!! so that $x_{n+1} = x(t_n+h) - x(t_n)$
$x_n = x(t_n)$] this is the further shift in thinking.

So that x is not really a function of n so much
furthermore as it is a function of time, & preferably incremental time in order to understand it as a differential equation. but how does this happen?

$$x(t_n+h) - x(t_n) = (a-1)x(t_n)$$

well, if $a = 0$, the solution of $x_{n+1} = ax_n$
which is $x_n = a^n x_0$
would be $x_n = 0^n = x_0$
or $x_n = x_0$
which is a useless, or trivial solution.
So this is the reason a cannot be equal to 1
but how would you know to do this if you did not know the solution?

So we see that
x is not just a function of n
but x is actually a function of t_n
This makes sense.

The discrete logistic equation is

$$N_{k+1} = N_k + R_0 N_k \left(1 - \frac{N_k}{K}\right)$$

N_k = Start number of population
R_0 = growth rate
K = a Constant
K & R_0 are usually detetermined experimentally)

The differential form is

$$\frac{dN}{dt} = \left(\frac{K-N}{K}\right) N R$$

	eg
N = Population number	10
R = Growth Rate	.01
K = a Coefficient	300

Slope field, online version, worked very well

with $y' = \frac{5-y}{5} \cdot 100 \cdot (.01)$

$$P = \frac{K P_0}{P_0 + (K - P_0) e^{-rt}}$$

$K = K$
$P_0 = N$
$t = t$

Actually, the derivative is
$y' = y \cdot (1-y)$

Ok, what we are actually doing is investigating the slope fields of a differential equation and also learning to formulate DQs.

We started out with

$y' = C$

$y' = Cx$

$y' = ky$ eg $y' = 9.8 - \frac{v(t)}{4}$

which became very interesting already.
You also learned how to use Math Studio to solve these, which was great!

You also started to learn about regressions in mathcad.

You also ~~started~~ to learn about DQ solution in mathcad but you see it is a lot more involved.

Math Studio looks like our easiest & most accessible tool.
But slope fields are even more fun.
And Math Studio is still best for <u>that</u>.

The System Simulator Program
seems to require that you set
$X' = X$ vs $X = 1$ in Math Studio?

In Math Studio, if you plot the slopes
you get the right results that make sense
System Simulator does not seem to give this

What if DSolve can not analytically solve
the DQ in Math Studio, what do you use?

Let's play around w/ some more examples.
How about
$y' = C$
It gave an immediate answer of
$y = -C_1 + Cx$ which is perfect.

Now try
$y' = Cx$
It immediately gives us
$y = -C_1 + \frac{Cx^2}{2}$ also correct.

This is great.
We can try lots of examples now.

We now also have
$y' = C - ky$
as
$$y = \frac{C}{K} + \frac{e^{-kx + C_1 K}}{K}$$

Which also
looks very good.

Math Studio has numerical solution for 1 ODE
RK4 & RK45

So now we have the solution to
$y' = C - ky$
as
$y = \frac{C}{k} + \frac{e^{-kx + C_1 k}}{k}$ let $C_1 = 0$ so

$y = \frac{C}{k} + \frac{e^{-kx}}{k}$ let $k = 5$
$C = .2$

There is a problem w/ the vector plots in mathstudio
You are having a problem w/ the vector plots.

Ok, some discoveries.
The vector field in Math Studio should be
expressed as

~~VectorPlot(f(x~~ VectorPlot(x, y')
not VectorPlot(1, y')
This means that it is now the same as the
dynamic simulator. Second the vector plot
(ie slope field) never gives you the full
solution with only one boundary condition

You cannot get a vector plot (slope field of the actual solution, only the slope of the solution.

Vector Plots do <u>not</u> use $y(x)$
They only use (x, y)

The Vector plots are <u>not</u> giving you the solution. They are <u>not</u> giving you the slope field.

There is a huge difference between

$$\text{VectorPlot}\left(x,\ 9.8 - (y/4)\right)$$

and

$$\text{VectorPlot}\left(x,\ 9.8 - \frac{y(x)}{4}\right)$$

Do you see it? You can pick any x, y but this is hardly the same as $x, f(x)$ or $x, y(x)$

You are not getting the slope fields

Vector input is apparently $\frac{\partial F}{\partial x}$ $\frac{\partial F}{\partial y}$

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So if $y = -39.2e^{-.25x} + 39.2$

$\cancel{\frac{dy}{dx}} = e^{-\cancel{.25x}}$

$\cancel{\frac{dx}{dy}} = 0$

$de^u = e^u + c$

$\frac{de^u}{du} = e^u + c$

Final Solution: y does equal a function of x only, not y.

You are not getting to slope fields

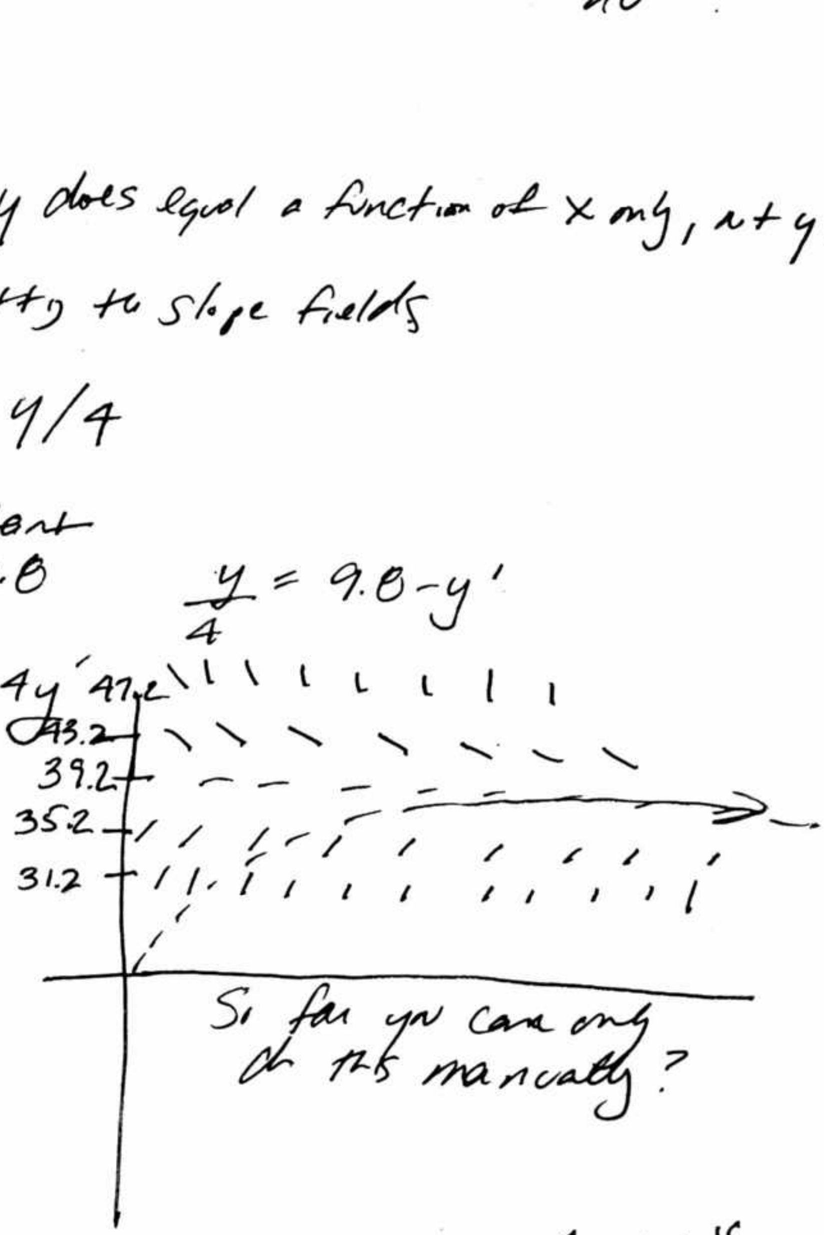
$y' = 9.8 - y/4$

Set y' = a Constant

$-\frac{y}{4} = y' - 9.8$ $\qquad \frac{y}{4} = 9.8 - y'$

$y = 39.2 - 4y'$

y'	y
0	39.2
1	35.2
-1	43.2
2	31.2
-2	47.2



So far you can only do this manually?

I have an answer on with an online tool @ mathscoop.com. It works great.

This is better

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You do not have a good offline tool yet.

Octave:
Define a DE with

`f=@(t,y) t*y^2` for $y'(t) = ty^2$

`[ts,ys] = ode45(f,[-2,2],1)`

`plot(ts,ys,'o-')` for $y(-2)=1$

`dirfield(f,-2:0.2:2,-2`

does not work yet, need more study.

For now, use online direction-field.

The logistic equation is also of the form

$$y' = y(1-y) \qquad = y - y^2$$

Math Studio appears to have a problem

$$\frac{dN}{dt} = \left(\frac{K-N}{K}\right)NR = \frac{1}{K}\left(KNR - N^2R\right)$$

$$= NR - \frac{N^2R}{K} \qquad = N\cancel{\frac{(R-N)}{K}}$$

So yes
we see they
are essentially
the same.

$$= \cancel{C\cdot N_0}\ C\cdot\cancel{\frac{y(K-y)}{K}}$$

rate of growth

$$= N\left(R - \frac{NR}{K}\right)$$

$$y' = y\left(r - \frac{y\cdot r}{C}\right)$$ Check this.

$$\frac{dy}{dx} = \left(\frac{K-y}{K}\right)y\cdot r = \frac{Kyr}{K} - \frac{y^2 r}{K} = \frac{r}{K}\left(Ky - y^2\right)$$

$= \frac{ry}{K}(1-y)$ and $\frac{r}{K}$ is indeed a coefficient

so essentially

$$y' = Cy(1-y)$$

eg $\frac{.02}{100}$ this does not match?

You have a stable solution @ $C = 3$ @ $y_0 = 0.6$ very interesting.

You have found an alternative
stable solution to the logistic equation.

$y' = cy(1-y)$

$y_0 = 0.6$

$y =$ ~~0.7~~ 7.0 does not work @ all

0.7 works

$c = 3$

$c = 3.5$ even more interesting
leads to a stable oscillating solution

@ $n = 500$ $y_n = .656$
$y_{n+1} = .677$

So it is slowly converging.

c should equal $\frac{r}{K}$ but this is making no sense?
I do not understand how $\frac{r}{K}$ can be equal to 3.

Stable from $y_0 = .01$ to $.99$
This means most any population.

$c = 2$ straight line $y_{n+1} = 0.5$
$c =$ ~~0~~ $4 \Rightarrow y_{n+1} = 0$
So $c = 3$ is about right

$c = 3.5$ is even more interesting.

3.6 is even more complex
3.7 also
3.8
3.9 gives a lot of variation
3.99 is very complex.

and yet it is 100% determinate
You could never figure out the pattern.

It oscillates between essentially 0 & 1

It does have a bias in it.
Notice when it reaches the bottom
it bounces back immediately but not the top
3.5 is much more stable.

3.6 is much more balanced.

So

$y' = Cy(1-y)$ $y_0 = 0.6$

Any relationship?
between 3.5 & 0.6
$6(0.6) = 3.6$?

$3 < C 4$

Web Plot shows the asymmetry

3 is perfectly stable
3.1 introduces asymmetry
2.9 very quickly stabilizes or at least
much more smoothly.

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The 0.6 is not critical
0.55 works also
0.5 works
.4 OK
.3 very stable
.8
.99 OK

It can be separated & partial fractions used.

It works between 0.01 & 0.99
so 0.5 is the midpoint.
looks like the stable is 3.0 & 0.5

Yes, this looks like a perfectly stable system.

$y' = 3.0y(1-y)$ and $y_0 = 0.5$

I wonder why this ratio?
There actually remains some asymmetry in the graph. It is skewed higher

Now, what if we use these parameters in Math Soft in a DQ?

It is interesting w/ math studio I get an implicit result. Why?

It doesn't look to me like mathsoft can solve it.

This is then a case for mathcad.
Maybe this is a nonlinear ODE?

The solution of the logistic equation is:
by Casio form

$$y = \frac{c}{1+ae^{-bx}}$$

It is a simple first order non linear differential equation.
Partial fractions are used after separation.

In your recursive work, you are actually using what is called a

"logistic delay equation" which has "rich" behavior.

You have to be careful w/ machine solutions.
Mathsoft seems to be having major difficulty.
Creating hyperbolic cosine & sine?
Clearly mathsoft cannot handle this.
I wonder if mathcad can?

Either way $y' = cy(1-y)$

One book says it is linear & the other says it is non linear.

So $y' = \frac{dy}{dt} = cy(1-y)$

$$\boxed{\frac{dy}{cy(1-y)} = c\,dt}$$

So this is separated, but it can not be integrated directly & apparently this is what partial fractions are about.

I say non linear.

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DQ

An equation is non linear if the variables or its derivatives are non linear. This is satisfied by

[redacted]

Jan 25 2015

What we see here is that Mathcad cannot really solve ODE's symbolically. It appears to involve only those that are immediately integrable.

I suspect Mathsoft is of the same ilk, it seems to be able to handle some simple cases but I am not sure how far it can go.

You basically need to solve it before these packages can likely solve it. Numerical solution is another matter, this seems to always be approachable.

The most instructive feature does seem to be slope fields. These are of immediate value no matter how complex the solution is. You have an online method for that, you have no offline methods as of yet.

227,11B

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Jan 26 2015

Analysis
Interpretation
& Use

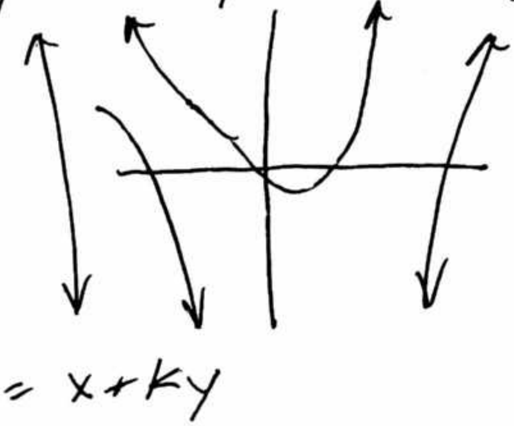
1st Tutorial:
1. Greenhouse Gases
2. Aerosols
] & Output

2nd Tutorial:
1. Long Term Effects Output
2. Random Effects Input
3. Mortality Output

DQS:
OK, where are we?

online slope generator is probably our most useful tool to start learning effects of factors

$y' = c$
$y' = x$
$y' = y$
$y' = ky$
$y' = x + y$ is interesting already



$y' = x + y$

$y' = x + ky$

What does it mean $y' = x + y$
change in y is proportional to y but also a linear function of x or time

eg

Change in Temperature is proportional to temperature itself but it is also a function of time so both of these influence are acting together.

A system of equations means it is acting in 2 or 3 dimensions, eg the change temperature of the atmosphere is proportional to the existing temperature but also a function of height (eg x or y depending upon direction)

So example, you put a red hot body into the atmosphere at 20,000 ft. we know that temperature of air alone is a function of height (this is equatable to "x") ie, position. But we also know that it is a function of the temperature difference ~~they~~.

eg
$$\frac{dT}{dh} = C_1 e^{-kh} \qquad h = \text{altitude}$$

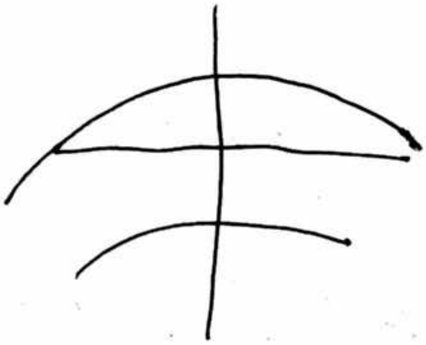
but we also know that
$$\frac{dT}{dh} = K\left(T_{body} - T_{air}\right)$$

so in this case
$$\cancel{\frac{dT}{dh} = K\left(C_1 e^{-k_2 h} - T_{air}\right.}$$
$$\frac{dT}{dh} = K\left(T_{body} - C_1 e^{-k_2 h}\right) = f(x, T)$$

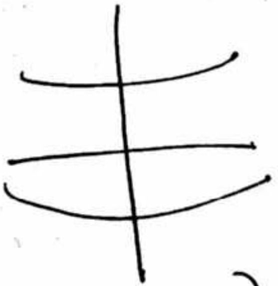
This is actually a better result.

A very "cool" example, get it?

$y' = e^{-ky}$



$y = e^{ky}$

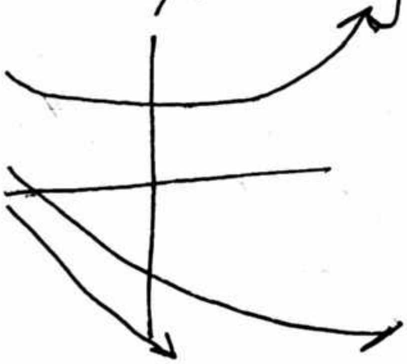


$y' = k_3(ky - e^{-k_2 y})$

3 coefficients
so 3 ~~non~~ linear equation
needed.

This is indeed very interesting.

This is
really really
interesting.



$K = 0.1$
$k_2 = -.05$
$k_3 = 0.8$

You can see
now how you can shape a DQ to
most any thing you want.
This is very <u>practical</u>.

Lets pick some number and see
how DPLOT does.

This is a wonderful edxample.

Lets keep going: keep using ΔT & h as an inspiration.

$y' = f(x^2 - y^2)$

A board is falling through the air parallel to the ground. As it falls it is subject to gravity.

$\frac{dV}{dt} =$ ~~$c\cdot V(t)$~~ $c\cdot t$ because acceleration is a constant so velocity is a linear function of time

but we also know that the resistance to velocity of the board is proportional to the area of the board of the velocity: This is leading to the square

$$\frac{dV}{dt} = -kV^2$$

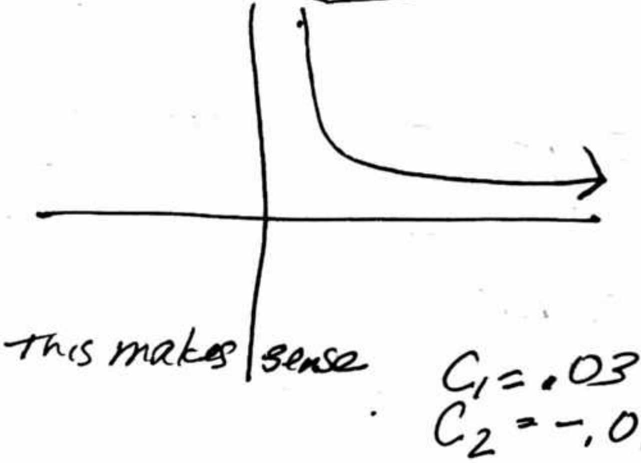
so doesn't this mean

$$\frac{dV}{dt} = c\cdot t - kV^2$$

you are trying to solve with wrt t

$$\boxed{y' = C_1\cdot x - C_2 y^2}$$

ie, the wind resistance of a board is much greater than that of a ball



This leads to a very quick reduction in V w.r.t. time

This makes sense

$C_1 = .03$
$C_2 = -.01$

So you definitely see how the DQS
Can now start to be formulated.

This is great
You can always get a numerical solution
or a regression approximation
if you want it.

Question: Can you solve these two
type of question explicitly?

Math Studio:

OK $y' = C_1 x$ $\quad y = C_1 \frac{x^2}{2}$

$y' = C$ $\quad y = C_1 x$ OK

$y' = Cy$ $\quad y = e^{C_1 x}$ OK

$y' = x + y$ $\quad y' = -x + e^{x} - 1$ Interestingly
looks OK

Implicit result $y' = y - e^{-y}$ looks like difficulty here

$y' = e^{y(x)} \Rightarrow y = -\ln(-x+1)$ looks ok

$y' = e^{C_1 \cdot y} \Rightarrow y = \frac{-\pi i}{C_1} - \frac{\ln(C_1)}{C_1} - \frac{\ln\left(\frac{-1}{C_1} + x\right)}{C_1}$

getting complicated
but not necessarily impossible

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$y' = C_1 x - C_2 y^2$

Definitely cannot be solved w/ Mathsoft but slope plot immediately shows the form of the solution.

We have a very nice slope field w/ $C_1 = .03$, $C_2 = -.01$

Lets thing about constructing a specific curve?

$$\frac{dV}{dt} = C_1 t - C_2 V^2$$

g when $t = 0$, $V = 0$ so $dV/dt = 0$

t	V	dV/dt	
0	0	0	
10	?	.3	$.3 = C_1(10) - C_2 V^2$
20	?	.5	$.5 = C_1(20) - C_2 V^2$

$C_2 V^2 = 10C_1 - .3$

$C_2 V^2 = 20C_1 - .5$

$1 = \frac{10C_1 - .3}{20C_1 - .5}$

$20C_1 - .5 = 10C_1 - .3$

$10C_1 = 0.2$

$C_1 = .02$

$C_2 = -\frac{.10}{V^2}$ @ $t = 0$

$C_2 = \frac{-.10^2}{V^2}$ @ $t = 20$

This is interesting

We know that

$$\frac{dV}{dt} = .02t - \underline{C_2} V^2$$

but now what.

@ $t = 20$, $\frac{dV}{dt} = .5$

If we have

$$\frac{dv}{dt} = .02t - C_2v^2$$

and we know that @ $t=20$, $\frac{dv}{dt} = .5$

we should be able to solve for C_2

$$-C_2V^2 = \frac{dV}{dt} - .02t$$

$$C_2 = \frac{\frac{dV}{dt} - .02t}{-V^2}$$

$$C_2 = \frac{.5 - .02(20)}{-V^2} = \frac{0.10}{-V^2}$$

so

@ $t=20$

$$.5 = .02(20) - \frac{.10}{-V^2}V^2$$

$.5 = .40 + .10$ and this is <u>true</u>.

Now what do you do w/ this?

We must need another set of conditions.

We know that $C_2 = \frac{.10}{-V^2}$ @ $\underline{\underline{t=20}}$

We know that $\frac{dV}{dt} = .02t - C_2V^2$ always.

We start with $f'(y) = f(x,y)$

We know that @ $t = \overset{50}{\cancel{100}}$, $\frac{dV}{dt} \approx$ ~~14~~ 10

$$10 = .02(50) - C_2 V^2$$

$$C_2 = \frac{9}{-V^2} \text{ @ } t=50$$

This is very interesting. I am not sure how we get C_2. C_2 is a constant, not a variable.

$$C_2 = \frac{.10}{-V^2} \text{ @ } t=20$$

The only thing solid we have is that

$$\frac{dV}{dt} = .02t - C_2 V^2$$

We also know that

$$C_2 = \frac{0.10}{-V(t)^2} \text{ @} t=20$$

or

$$C_2 = \frac{0.10}{-V(20)^2}$$

So we do know something. Remember you do not know V. But obviously if you assume that you do know V(20) then you know C_2

lets say V(20) = ~~10m~~ 5 m/sec.

then $C_2 = \frac{.10}{-5^2} = -.004$

this says

$$\frac{dV}{dt} = .02t - .004V^2$$

This defines V.

So $V(0) = 0$

$V(20) = 5$

These conditions should define V.

This by itself produces a slope field.

I think you have to numerically integrate this to find the specific form of V since you cannot actually solve it.

Don't feel bad. MathStudio cannot solve it either.

We can also see from the slope field that the limit of our solution approaches ~10 @ $t \to \infty$.
This is interesting also. How do we use this?

What we really have is that

$$\frac{dV}{dt} = .02t - .004\,V(t)^2$$

We know that $V(0) = 0$
$V(20) = 5$ m/sec
$V(\infty) \to 10$ m/sec

You keep thinking that there is a closed form for this solution, but not necessarily.
Just because the slope hase this form doesn't say anything about the form of the solution.

This is very cool. Runge Kutta 4 in MathStudio does indeed give a very good looking solution. Simple & to the point.
The limiting velocity in this case appears to approach 10.98 m/sec.

A step size of 1. gives the same result as a step size of 0.1
We really do have a decent solution
The step size is not really the step size.
10 values are sufficient.

This means we now easily come up w/ a closed form regression solution w/ the 10 points.

Notice the solution is not really bounded.
Believe it or not, Logistic Solution is obviously the best here.

$$V = \frac{12.48}{1 + 40.486e^{-.1385t}}$$

Mean square error = <u>.053</u>

This actually is quite decent.
This tells us that we have a limiting value at 12.48 m/sec
This is really quite reasonable and you have formed

What is interesting is I thought this numerical solution might be logarithmic but indeed it is very characteristically logistic. It is actually a marvelous fit.
I think your model is sound.

Jan 21 2015

We see now that the model for a flat board falling is not exactly realistic.
the model

$y' = C_1 x - C_2 y^2$ has a problem in that it does not seem to converge

the square term, if too large turns the velocity negative or slows it down, which is not possible.

It can suffice for an interval of time but not as $t \to \infty$.

Seems to me you need to subtract an exponential or log term.

Numerical Integration works great.
Let's try logistic

$y' = \left(\frac{K-y}{K}\right) \cdot y R$ let $K = 300$, $y(0) = 10$, $R = .01$

ie
$y = f(x)$
or $y = f(t)$
$N = f(t)$

Worked very well w/ RK4 w/ Math Studio.

$$y \cong \frac{300}{1 + 29.02 e^{-9.98t}}$$

This should actually work very well for the wind resistance problem translated is

$$\frac{dV}{dt} = \left(\frac{K-V}{K}\right) \cdot V \cdot R = C_1 V\left(1 - \frac{C_2}{C_1} V\right)$$

$$\boxed{= C_1 V(1 - C_2 V)}$$

This is a more general form.

$$= \frac{1}{K}\left(KVR - V^2 R\right) = \frac{R}{K}\left(KV - V^2\right)$$

$$= C_1\left(C_2 V - V^2\right) = C_1 V - C_2 V^2 = V(C_1 - C_2 V)$$

So the more general form of the logistic equation is

$y' = C_1 x(1-C_2 x)$ This is indeed a logistic form.

We have $C_1 = 2E-4$
$C_2 = 1E-3$

and we did not see the logistic form kick in until x approaches 1000.
But it did work very nicely
Notice this is y' NOT Y!

Graphing this equation (slope field) is very interesting. C_2 makes a big difference. $C_2 = 0.1$ introduces the logistic style. As C_2 increases it causes the population to decline.

C_1 is what causes the increase rate
C_2 is what tailors the decline rate.

Increasing x causes a big difference. We have a graph of $x_{max} = 80$
$y_{max} = 200$
w/ $C_1 = 0.2$ and $C_2 = 0.015$ that demonstrate the slope well
It has become much more interesting w/ the form

$$y' = \sin(t)\left(C_1 t(1-C_2 t)\right) \quad \text{w/ } C_1 = 0.2,\ C_2 = 0.015$$

look@

$$y' = C_3 \sin\left(\frac{t}{y}\right)\left(C_1 t(1-C_2 t)\right)$$

$(t \cdot y)$

I have maxed out the system.
Very exotic behavior possible here

Feb 4, 2015

Page 32

It is time to start getting organized again. There has been a hiatus from CA trip & illness. There are many factors on the table:

1. CI Work
Edvotek Work
Chromatography
IR Anyway?

CI
2. Research
Climate Model:
Video & Paper
Longevity Model
Chemistry of Oils
Tesla Read

[redacted]

4. Personal
Patterns
Food
Innovative
Amazon Purchase

5. Math Studies

Calculator Investigations
MathCad Investigations
Recover Exp Harmonics
Recover Probability
Diff Equations
Dynamic Systems

6. Lab Work
1. Edvotek
2. Metabolic API
3. Chromatography Lipids
4. IR Lipids
5. IR Proteins

7. Ham Radio

8. Accounting

9. Modeling
Longevity Model?
Climate Video?
Climate Math Paper?

10. CI Purchases
Batteries
Paper

Video Outline

Outline of Climate Model Video

Model has the following Components:

Inputs:
1. GH gases + & −
2. Aerosols (9 types + and −)
   No of operation
3. Random Events

Output:
1. Immediate or Short Term Heat Response
    1. Magnitude
    2. Direction
    3. Time

2. Long term effects relative
   to a reference frame of 1 & 5°

Translated Changes
   Crop losses & Ice Ages

3. Mortality Estimates infections
   (Disregarding health & biological
   aspects)

Video Outline

Comment on Various Sectors
Historical Perspective:
1. ~~GH gases~~: Climate as a whole is changing
Kirsten Peters. & Geologist perspective.
Perspective required.
Milankovitch
~~2. GH gases~~ Geologists.

2. GH Gases
Scale of Magnitude
Political focus on taxation strategies
Activist strategies on alarmism.
w/ avoidance of more ~~to~~ likely source
Causes such as geoengineering

Mitigation Strategies
Known reduction of methane
Alarmist scenario of a methane
albeit possible but not supported by recent trends
of 25 years.

Coal & Natural gas line

Same as methane can be accomplished

Elimination of CO_2 is not the goal
or else we do not have plants or oxygen
Sign of Oxygen

Video Outline

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Aerosols.

1. Overall effect of almost all aerosols is to heat the planet.

2. High Clouds also heat.

Nature of aerosols + geoengineering to cool the planet under any current incarnation is a fraud.

3 Authoritative sources validate the results of this model.

1. CERN
2. Pnas
3. IPCC

] Credit to Chemtrails Planet.net

Now Consider Combined Effects of GHG & Aerosols.

Point: It is predictable whether we will have a net heating or cooling effect.

Effect upon health of planet Can not be ignored when aerosols are introduced.

Video Outline

1. Random Event Discussion

Stability & Instability

2. We should be talking about long term implications & what are we actually doing as to ensure survivability of the species?

3. Other aspects / Biological & Energy

4. Conclusion

If there is any doubt that geoengineering can be implemented and that it has consequences upon the planet all that is needed is to evaluate the factors that have been incorporated into this model.

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CDC data

Median Income K	Mortality per 100,000
12K	1000
18K	800
24K	600
34K	400
55K	300
85K	200

$y = ax^b$

$y' = bax^{b-1}$

I have a perfect graph

$y = 8466.05 \cdot \text{Income}^{-.8417}$

Mortality per 100000

$r^2 = .991$

mse = 4.10E-3

y is $\frac{\text{Mortality}}{\text{per } 100{,}000}$

$y = \frac{dM}{\cancel{dN}}\, \underline{dI}$

1,000 per 100,000 = 1%

$\frac{dy}{dI} = -7125.9 \cdot \text{Income}^{-1.8417}$

9

1240 people died between 10 & 11K $

270 people 60 & 61K

4.6

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What we need next is the probability of dying as a f(age)

We have a first function of

Prob Dying $= .01464 + .001346e^{.05518t}$

t in years

The social security data is too conservative.
It represent the probability of dying within a year but not the cumulative probability.

I think it needs to be normalized

So
1. Take SS data
2. Integrate it
3. Normalize it.
4. Curve fit it
5. Cum Probability of Death $= -.0064 + .000274e^{.0693t}$

t in years

$r = .999$

age	Pr(death)
20	~~1.9%~~ [illegible].5%
40	
60	
65	
70	
75	
80	
85	
90	
100	
110	
120	

Pase 39

@ 100 = x   14 = 4.423

years	Pr(death)
0	0
10	0
20	.4%
30	.4%
40	.6%
50	1.4
60	3.0
62	~~6.8~~
65	
70	6.8
72	
80	17.1
90	47.4
100	100%

This approach is interesting.
Say we had $\bar{X}$ = ~~76.8yrs~~ 76yrs = 11.7%
So say we have a pct chance increase in death ~~from lower income~~. a 100% increase. = 23.4%
≅ 83yrs
76 - 83 = -7 years
76 - 7 = 69 years!

This is very reasonalble.

Median household income

$= \$35,371$

Our Mortality Rate Function is

$MR = 8466.05\ \text{Income}^{-.8417}$

(mortality rate per 1000)

Average $MR_{35.4K} = 420.9$

~~Median~~ Mortality Rate = 420.9 per 1000

Next we compute the MR for Income = 15,000

$MR_{15K} = 866.5$

$\% \text{ Increase} = \frac{866.5 - 420.9}{420.9} = 105.9\%$

At the average life expectancy 76 yrs
Pr) mortality $\cong 11.7\%$
Cumulative

It really could be ~~less~~ greater than this. But a Conservative approach

$(1 + 1.06)(11.7\%) = 24.10\%$

This corresponds to an age of 83 years

$76 - 83 = -7$ years $\Rightarrow$ 69 years

In reverse, if you make 60k per year.

$\frac{269.8-420.9}{420.9} = -35.9\%$

$(1-.359) = (.64)$

$.64(11.7) = 7.5\%$ $= 71$ years

$76 - 71 = 5$ years

$76 + 5$ years $= 81$ yrs.

Now let's figure out the reverse relationship on advance:

Instead of using

$1+\Delta MR$ it should be $\frac{1}{1+\Delta MR}$

g: $\frac{11.7\%}{1+1.06} = 5.68\%$ ⇒ 67 years. much more realistic

$\frac{11.7}{.64} = 18.3\%$ ⇒ 81 years good.

This work looks very good.

You have something here that already makes sense.

We have a good equation

$\text{CumMortalityRate} = -.00252 + .0001989e^{.08602t}$

t in years.

@ $t=76$, $y=\underline{13.5\%}$

$r = 0.\underline{998}$ this works fine

Ok, we already have a handle
on ~~est~~ income.
How about heath insurance.

With respect to health insurance
we have a first estimate of

40% to an 80% hazard increase.

$$\frac{Pr_{76} \ (=13.5\%)}{1+.60} = 8.44\%$$

≅ 10.9 years

Women go from
17% to 10%

76 - 10.9 yrs = 5.1

So you earn 15K w/ no health
insurance
life expectancy is ~ 66 years vs 76 years.

We need sex
education
income
insurance

We have info for education also.

[redacted]

Now look @ education

			+25			
	M	F	M	F	M	F
<HS	44	50	69	75	-7	-6
HS	51	56	76	81	0	0
Some College	52	58	77	83	+1	+2
College	57	62	82	87	+6	+6
Graduate Deg.	60	62	85	87	+9	+6

These numbers are very sensible.
Now quantify them.

This can just be a table format.

Factors are
1. Sex
2. Income
3. Education
4. Health Insurance

Smoker?
Overweight?

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We have normalized P(r) mortality curves of form:

$$P(r) = a + be^{C\cdot years}$$

will have a Pr and we need to solve for years

$$be^{C\cdot years} = P(r) - a$$

$$e^{C\cdot years} = \frac{P(r)-a}{b}$$

$$C\cdot years = \ln\left(\frac{P(r)-a}{b}\right)$$

$$years = \frac{1}{C}\ln\left(\frac{P(r)-a}{b}\right)$$

We can not have the log of a negative number

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Practical Application of a DQ.
Tannenbaum p 133
#1

[redacted]

$\frac{dP}{dt} = kP$ $\qquad \frac{dP}{P} = k\,dt$

$\boxed{3\ 4}$
1 8

Do - to
Do Actions 8

$\int \frac{1}{x}\,dx = kt$

$\ln x = kt + c$ $\qquad x = e^{kt+c_1} + C_2 \Rightarrow y = e^{kt+c_1} + C_2$

$y = e^{kt} \cdot e^{c_1} + C_2 \Rightarrow y = C_1 e^{kt} + C_2$

let $y = \underline{1}$ @ $t = 0$
$y = 2$ @ $t = 50$

$y = e^{kt} + \cancel{C_2}$

$2 = e^{k \cdot 50}$ $\qquad \ln(2) = k \cdot 50 \quad k = .01386$

$y = e^{.01386t}$ $\qquad 3 = e^{.01386t}$ $\qquad \ln(3) = .01386t$

$t = 79.26$ days $\quad \underline{\text{good}}$

This was solved properly.

[redacted]

Open office 1.4

$\underline{\underline{\text{SXW}}}$

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[redacted]

— Star Office

ODT

[redacted]

Open Office

(Libre)

HTML5

Libre

[redacted]

Lets try to formulate a df eq.
A simple one.
Start thinking about small changes in x & y

$y = f(x)$

The case of

$\frac{dI}{dx} = CI$ was one case.

but he did not want it in terms of I
he wanted in terms of Amplitude.

$I = \underline{CA}^2$ Now what is implicit differentiation?

What exactly is an implicit function?

An implicit function is one in which the dependent variable IS NOT ISOLATED on one side of the equation.

$$\frac{dv}{dt} = \frac{dv}{ds}\frac{ds}{dt}$$

The Chainrule and the product rules are really quite profound, as they eventually affect what implicit diff is all about.

Chain Rule if $y=f(u)$ and $u=g(x)$
then $\frac{dy}{dx} = \frac{dy}{du}\frac{du}{dx}$ this is really quite amazing when you think about it.

Example:
$y=f(u)$ eg $y=u^2$
but remember $u=g(x)$ so let $u=x^2+1$
so

$$\frac{dy}{dx} = \frac{dy}{du}\frac{du}{dx} \qquad \frac{dy}{du} = 2u$$

so

$$\frac{dy}{dx} = 2(x^2+1)\cdot 2x \qquad \frac{du}{dx} = 2x$$

This is the Chain rule form. They both lead to the same result.

We could also have said $y=(x^2+1)^2$ This is the power rule form
so $\frac{dy}{dx} = 2(x^2+1)(2x)$
and yes, you have the same result.

Now lets go back to implicit diff. (ie y is not isolated) $\underline{y}$.

$$y^4 + 3y - 4x^3 = 5x + 1 \quad \text{Find } \frac{dy}{dx}$$

First we recognize that it is an implicit function.
Also y means $y(x)$

So study implicit diff further:

$y^4 + 3y - 4x^3 = 5x+1$ So this is implicit.

and this really means

$f(x)^4 + 3(f(x)) - 4x^3 = 5x+1$

and if the two sides are equal then y' is equal

$D_x(f(x)^4 + 3f(x) - 4x^3) = D_x(5x+1)$

So

$4f(x)^3 f'(x) + 3f'(x) - 12x^2 = 5$

$f'(x)(4f(x)^3 + 3) = 5 + 12x^2$

$f'(x) = \frac{5+12x^2}{4y^3+3}$ or $y' = \frac{5+12x^2}{4y^3+3}$ good

This is great. We have this correct.
What you realize is that this **IS** a diff equation.

a huge lesson here. Any isolated derivative
regardless of how simple or complex
does represent a differential equation.

This was a great lesson!

Lesson: The derivative of anything represents a differential equation.

Try to give meaning to all differential form ~~that~~ you view now.
Also try to formulate them.

Notice in the original equation that you could not solve this for y. at least not explicitly. But notice that when you differentiated it you were indeed able to solve it for y'. Since you solved it for y', with an initial condition you were able to solve for y = f(x) and x alone. This is fascinating. Something that you never would have been able to do you were able to do by looking @ it from the standpoint of a diff eq !!

* * * !!!

These were surprising lessons:

1. The actual definition of an implicit function
2. How to implicitly differentiate w/ clarity
3. In this case, how to isolate y'
4. The ~~important~~ realization that y' IS A DIFFERENTIAL EQUATION!
5. The ~~non~~numerical solution of the DQ with a result essentially of y = f(x) alone which you never could have gotten to otherwise.

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Another thing you see here is that there is infinite variety of form w/ DQS.
It would be wonderful to be able to formulate them.

Q:
1. It rains. When does the drain max capacity?
2. A bacteria grows but then slows down & stops. Why & when?
3. What is the length of a shadow as a function of time?
4. How much does a car tire wear down?
5. When does the temperature of a room equalize?
6. How much force did it take to start my wind vane
7. How fast does my wind vane turn?
8. A bullet in water

rate of change
increase
loss
decomposition
growth
decrease

these are all flags to be DQS.

9. The terminal velocity of a parachute
10. Stopping distance of a car w/ brakes.

This is not so obvious.
You have to think it through.

Your book by Tenenbaum is nothing less than a 'journey of practicality'.

DO

Hundreds of equations are formulated in the book all the way through systems of equations & even Bessel functions

The a great study material

$F = m \cdot a$

$F = m \cdot \frac{dv}{dt}$

we really want to work this one through to understand it.

In terms of Frictional force

$F = m \cdot a - \mu m a$

The original law was actually

$F = K \cdot m \cdot a$

There is actually a proportionality constant involved.

$F = K \cdot m \cdot \frac{dv}{dt}$

We know in SI units that $\frac{dv}{dt} = \frac{9.8m}{sec}$

$F = K \cdot m \cdot \frac{9.8m}{sec}$

Maybe it should be $\frac{dv}{dt} = \frac{F}{K \cdot m}$

$\frac{dv}{dt} = \frac{dv}{ds}\frac{ds}{dt}$ Chain rule.

and $\frac{ds}{dt} = v$

so

$\frac{dv}{dt} = v \cdot \frac{dv}{ds}$ and $F = m\frac{dv}{ds}$

We are ok with.

$m \cdot a = -9.8\, m$

^ $a = -9.8$ m/sec OK This is vertical motion

or $\frac{dv}{dt} = -9.8$

Ok, we are ready for horizontal motion now.

Frictional force = $\mu m \cdot g$

Frictional force = $\mu \cdot m \cdot \frac{dv}{dt}$

$\frac{dv}{dt} = \frac{dv}{ds}\frac{ds}{dt}$

This means that we also have

Frictional Force = $\mu \cdot m \cdot \frac{dv}{ds} \cdot v$

and

$\frac{dv}{dt} = \frac{dv}{ds} \cdot v$

g

$10 kg \cdot 9.8 \frac{m}{sec} - 2 \cdot v = \mu \cdot 10 kg \cdot \frac{dv}{ds} \cdot v$ or $\left(\frac{dv}{dt}\right)$

$m \cdot a = 10 - 2v$

Net Force = Pulling Force − Air Resistance

This is the heart of the relationship.

yes this is true.

Another source had

$F = ma$ but F is the sum of forces

so $(F - f) = ma$

F = pulling force

f = friction

This is the same as we have above.

It should not matter what the units are

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This leads to

$$m \cdot \frac{dv}{dt} = 44.5(N) - 2v$$

1 "pound" = 4.45 Newtons
1 "pound" = .454 kg.

$$\frac{dv}{dt} = \frac{44.5 - 2v}{29.06\,kg}$$

✓ we need this to be about 25V to match the book. why?

64 pounds ~~force~~ wgt = 29.06 kg
10 pounds force = 44.5 Newtons

@ 5 sec, v ≐ ~~7.1~~ 6.5 m/sec

The terminal velocity appears to be ~ 22.1 m/sec
The solution looks very good but we does not agree w/ the the book answer. They get @ t=5 v ≐ 5.0 ft/sec
We are not close to this. Why?

64 pounds wgt
10 pounds force

assume no friction.

64 pound weight = 29.06 kg.
10 pounds force = 44.5 newtons

$$(F - f) = ma$$

$$44.5 - 2V = 29.06\frac{dv}{dt} \Rightarrow \frac{dv}{dt} = \frac{44.5 - 2v}{29.06}$$

I do not see any mistake here.

Mathstudio gives us

$$V = \cancel{84}\ \frac{89}{4} - \frac{89}{4} e^{-.0688t}$$

$$V = 22.25 - 22.25e^{-.0688t}$$

$V(5) = 6.5$ So my results are correct if my units are correct.

terminal velocity = 22.25 m/sec

Limit definition

$$f'(x) = \frac{f(x+h) - f(x)}{h}$$

so it is a ratio of $\frac{\Delta y}{\Delta x}$

eg x^2 @ $x=3$

$$\cancel{x} \quad \frac{(3+.001)^2 - 3^2}{.001} = 6.001$$

Sure enough

Related Rates.

P194 Skokowski

$$x^2 - y^3 - 2x + 7y^2 - 2 = 0$$

Now in this case $x=f(t)$ and $y=f(t)$

$$D_t(x^2 - y^3 - 2x + 7y^2 - 2) = D_t(0)$$

$$2x\frac{dx}{dt} - 3y^2\frac{dy}{dt} - 2\frac{dx}{dt} + 14y\frac{dy}{dt} = 0$$

$$-3y^2\frac{dy}{dt} + 14y\frac{dy}{dt} = 2\frac{dx}{dt} - 2x\frac{dx}{dt}$$

$$\frac{dy}{dt} = \frac{(2-2x)\frac{dx}{dt}}{14y - 3y^2}$$

$$\frac{\frac{dy}{dt}}{\frac{dx}{dt}} = \frac{2-2x}{14y-3y^2}$$

→ Doesn't this mean $\frac{dy}{dx} \overset{?}{=} \frac{2-2x}{14y-3y^2}$

Remember the chain rule

$y=f(u)$ then $\frac{dy}{dx}=\frac{dy}{du}\frac{du}{dx}$
$u=f(x)$

Related rates

An even simpler case:

$$x^2+y^2=400$$

$x=f(t)$, $y=f(t)$
but it actually is true that $x=f(y)$
and that $y=f(x)$
but we are saying that they also can become functions of $\underline{t}$ time

$$2x\frac{dx}{dt}+2y\frac{dy}{dt}=0$$

eg ~~$z=f(x,$~~ $y)$
$z=f(x)$ $x=f(t)$
then $\frac{dz}{dt}=\frac{dz}{dx}\frac{dx}{dt}$
This is where this comes from.

$$2y\frac{dy}{dt}=-2x\frac{dx}{dt}$$

$$\frac{dy/dt}{dx/dt}=-\frac{x}{y}$$

when $y=12$ eg
what does x equal?

We need to solve for x: $x^2=400-y^2$ $x=16$

so

$\frac{dy}{dt}=\frac{-x}{y}\frac{dx}{dt}$ $\Rightarrow$ $\frac{dy}{dt}=\frac{-16}{12}\frac{dx}{dt}$ and dx/dt is given @ $2\,\text{ft}/\text{sec}$

$$\frac{dy}{dt}=\frac{-16}{12}\cdot 2\,\text{ft}/\text{sec}=\underline{\underline{-2.67\,\text{ft}/\text{sec}}}$$

Indeed you can solve for the ratios of the slopes but it is even more [illegible] to find dy/dt when you know dx/dt.

This is not really a differential equation.

Our final relationship here was

$$\frac{dy}{dt} = \frac{-x}{y}\frac{dx}{dt}$$

This is worth studying what it truly means.

$$\dot{y} = \frac{-x}{y}\dot{x}$$

you have 3 things that are changing here: x, y, & dx/dt.
That is a lot to get a handle on.

$\frac{dy}{dt} = \frac{-x}{y}\frac{dx}{dt}$ would be a differential equation, but this is not. It is

$\cancel{\frac{dy}{dx}} =$ but what if:

$$\frac{\frac{dy}{dt}}{\frac{dx}{dt}} = \frac{-x}{y}$$

So what if we set

yes, this IS OK to do.

$$\frac{dy}{dx} = \frac{-x}{y}$$

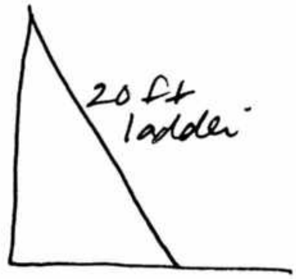
and this IS a diff. equation

This is actually a very interesting solution
Yes, this idea works perfectly
This does give you the equation of a circle!

Related rates are a very interesting approach
you needed to know the functional relationship
before you started. But what if you did not?

In our case, we knew we had a circle.
But what if we did not know?
What we really know is that $\frac{dy}{dx} = \frac{-x}{y}$

How would we know this?



when we move x a little,
how much does y move.

$$\frac{dy}{dx} = \frac{-x}{y} \Rightarrow \frac{\Delta y}{\Delta x} \approx \frac{-x}{y}$$

if you move x 20 ft to the right,
y drops 20 ft to the ground.

Δx	Δy	y'	x	Y
20	-20	-1	0	20
10	-10	-1		

you also measure this

This is what we measure.

x	y	Δx	Δy	$\approx y'$
0	20			
1	19.97	1	-.03	-.03
2	19.90	1	~~-.10~~ -.07	~~-.05~~ -.07
3	19.77	1	-.13	-.13
4	19.60	1	-.17	-.17

we see that it is $y' = -\frac{x}{y}$

but you only have
to have this.

it would not
be obvious that
this is a
circle.

This is all
that we will have

Think about this.
A car is accelerating.
you time the speed @ 1 sec intervals
How far has the car gone in 10 secs.

Water is flowing from a bucket.
You measure the rate
How long until it is empty?

The sun is rising.
You measure its angle.
When is it @ certain point.

1. Related Rates are very interesting forerunners of DQC.

2. Tennebaum is stepping through many DQ formulations

So a question is, what is the advantage of measuring the change vs measuring the function itself?

look @ $y=x^2$

actually $y'-1$

x	y	Δx	Δy	y' $(\Delta y/\Delta x)$	
0 .01	0 .0001	.01	.0001	.01 $\approx$ 0	0
1	1	1	1	1	2
2	4	1	3	3	4
3	9	1	5	5	6
4	16	1	7	7	
5	25	1	9	9	
6	36	1	11	11	
7	49	1	13	13	
8	64	1	15	15	
9	81	1	17	17	
10	100	1	19	19	

$y' = \cancel{x+1}\ 2x-1$

$0=(2x-1)+1$

$y=x^2+C$

$y=f(x)+C \quad C=1$

$y=\cancel{2x}\ x^2$

Notice the offset at 1.
Why does this happen.
It would be better to use $f(x+h)$

and here we can see $y'=2x$

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$y = x^3$

x	y	Δx	Δy	$\sim y'$	y'	y^2	y^3	y^4
0	0				0			
1	1	1	1	1	3	3		
2	8	1	7	7	12	9	6	0
3	27	1	19	19	27	15	6	0
4	64	1	37	37	48	21	6	0
5	125	1	61	61	75	27	6	0
6	216	1	91	91	108	33	6	0

$\sim y' \cong 2x - 1$

$\sim y' = 3x^2 - 3x + 1$

$y' = 3x^2$

$y' = 2x$

$\sim y' = 2x - 1$

$y' = 3x^2 - 3x + 1$

$y' = 2x$

$y' = 3x^2$

$y = x^2$

x	y	$\Delta y'$	Δy^2	Δy^3
0	0			
1	1	1		
2	4	3	2	0
3	9	5	2	0
4	16	7	2	0
5	25	9	2	0
6	36	11	2	0

$\Sigma D^n = \emptyset$ as $n \to \infty$ n = order + 1

$\Sigma \Delta y$

$y = \sin x$

x	y	y'	y^2	y^3	y^4	y^5	
0	0						
.1	.10	.10					
.2	.20	.10	0				
.3	.295	.095	-.005	-.005	~~.009~~		
.4	.389	.094	-.001	.004	.009		
.5	.479	.090	-.004	-.003	-.007	-.016	
.6	.564	.085	-.005	-.001	.002	-.009	.007

Notice this does not seem to be converging?

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$i^2 = -1$

$D^n = 0.$

what is $(-i)^2$

$= (-\sqrt{-1})^2$

$=$

$D^2 + D = 0$

$\lambda^2 + \lambda = 0$

$\lambda(\lambda+1) = 0$ $\quad \lambda = 0, -1$

$y = C_1 e^{0x} + C_2{}^{-xe} = C_2 e^{-x} + C_1$

$D^3 + D^2 + D = 0$

$\lambda^3 + \lambda^2 + \lambda = 0$

$\lambda(\lambda^2 + \lambda) = 0$

$= x(x^2 + x + 1) = 0$

0

$D^4 + D^3 + D^2 + D = 0$

$\lambda^4 + \lambda^3 + \lambda^2 + \lambda = 0$

why did you do this?

$x(x+1)(x^2+1)$

how did you even find the roots to these?
Why did you set it up as $\Sigma D^i = 0$?

$D^4 = 0$ make more sense.

$0, -1, i$

$0, -1, \pm i$?

$\lambda^3(\lambda+1) + \lambda(\lambda+1) = 0$

$\lambda^3 \cancel{(\lambda+1)} = -\lambda \cancel{(\lambda+1)}$

$-1, 0, i$

$\lambda^3 = -\lambda$ $\quad -1$

$\lambda^3 + \lambda = 0$

$\lambda(\lambda^2 + 1) = 0$ $\quad 0, i$

$x^2 = -1$

$x = i$

$1 - 1 + 1 - 1 = 0$ ok

0, ok

you have the heart of it.

$x^6 + x^5 + x^4 + x^3 + x^2 + x$

$= x(x+1)(x^2+x+1)(x^2-x+1) = 0$

$0, -1$

$x^2 + x + 1 = 0$ two roots

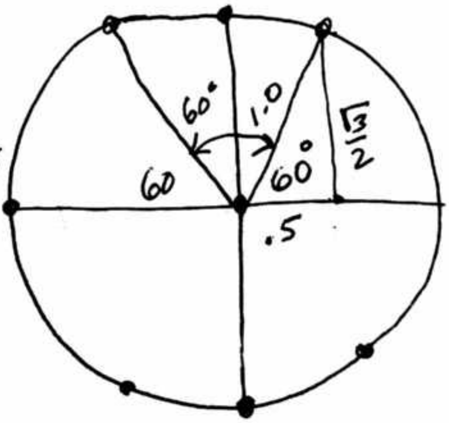
$x^2 - x + 1 = 0$ two roots

$-\frac{i\sqrt{3}}{2} - \frac{1}{2}$, $\frac{i\sqrt{3}}{2} - \frac{1}{2}$ $x^2 + x + 1$

$-\frac{i\sqrt{3}}{2} + \frac{1}{2}$ $\frac{i\sqrt{3}}{2} + \frac{1}{2}$ $x^2 - x - 1$

$0, -1$

This looks good. Easily found the roots



$x^4 + x^3 + x^2 + x = 0.$
$= x(x+1)(x^2+1)$

$0, -1, -i, i$

8 roots ok

/ $x^8 + x^7 + x^6 + x^5 + x^4 + x^3 + x^2 + x = 0$
$= x(x+1)(x^2+1)(x^4+1)$

$x^4 = -1$?

$\sqrt{2}\,(0.5 - 0.5i)$
$-\sqrt{2}\,(0.5 + 0.5i)$
$-\sqrt{2}\,(0.5 - 0.5i)$
$\sqrt{2}\,(0.5 + 0.5i)$

o/h
a/h
o/a

We already have the pattern

Roots are easy to solve w/ Math Studio

We have already recovered the roots of the solution.

Let's try an asymmetric solution.

$D^2 + D$ $\quad \lambda(\lambda+1) \quad = 0, -1$

~~$D^3+D^2+D = 0$~~

~~$= D(D^2+1) \quad 0, i, -i$~~

D^3+D^2+D

$\lambda^3+\lambda^2+\lambda = 0 \quad 0, \; -\frac{1}{2}+\frac{i\sqrt{3}}{2} \quad -\frac{1}{2}-\frac{i\sqrt{3}}{2}$

$D^4+D^3+D^2+D = 0 \quad 0, -1, i, -i$

$\frac{360}{5} = 72^\circ$ $\quad D^5+D^4+D^3+D^2+D = 0$

$-0.81-0.59i, \; -0.81+.59i$ $\quad 36^\circ$

$.31-.95i, \; .31+.95i$ $\quad 72^\circ$

0

$D^6+D^5+D^4+D^3+D^2+D = 0$

-1

60° $\quad -.5+.87i, \; 0.5-.87i$

0

60° $\quad -\frac{1}{2}-\frac{i\sqrt{3}}{2}, \; \frac{1}{2}+\frac{i\sqrt{3}}{2}$

51.4° $\quad D^7+D^6+D^5+D^4+D^3+D^2+D = 0$

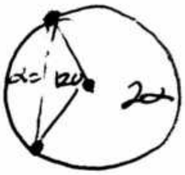
25.29 $\quad -.91-.43i, \; -.91+.43i$

$-.22-.97i, \; 0, \; -.22+.97i$

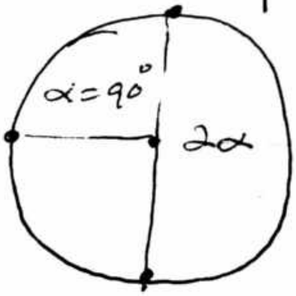
$.62-.78i, \; .62+.78i$

D=2

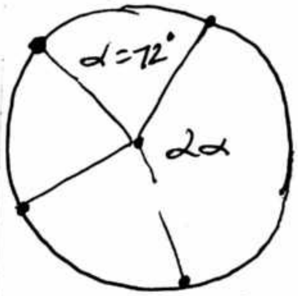
D=3



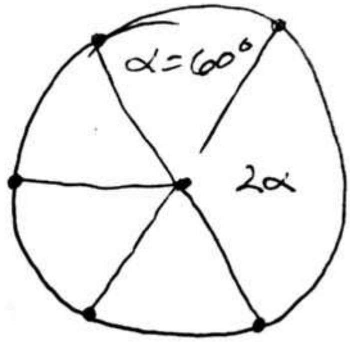
D=4



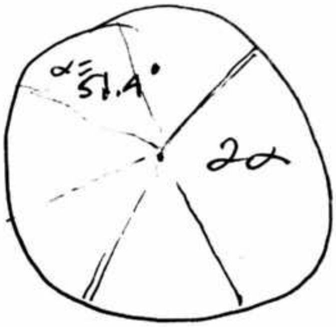
D=5



D=6



D=7



$(n-2)\alpha + 2\alpha = 360$

$n\alpha - 2\alpha + 2\alpha = 360$

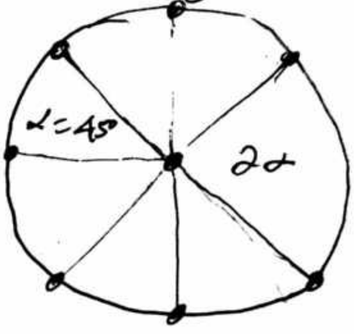
$\alpha = 360/n$

$\alpha = 51.4$

So you see the pattern.

Now, why did you propose that $\Sigma D^i \overset{?}{=} \emptyset$

D=8



$\alpha = 45°$

a cubic does appear sufficient

The sum does not equal zero, it equals a cubic

$ax^{n-1} + bx^{n-2} + \dots c$

$\Sigma D^n = ax^2 + bx + c$ almost perfect symmetry

Notice that it is zero @ the midpoint.

So it may be linear also

Lets start w/ a simple model

$D^2 + D = ax + b$ or $ax^2 + bx + c$

Lets solve this.

$y = C_1 + C_2 e^{-x} + f(x)$

The particular solution is going to be interesting because it will apply to only a minimal no of terms.

Assume y_p has form ~~$ax+b$~~ $A_1 x + A_0$ for now

$y' = \cancel{a}\, A_1$ This will not be hard!

& then this gets substituted.

and $y'' = 0$

$y'' + y' = A_1 x + A_0$

So

$0 + A_1 = A_1 x + A_0$ looks like it does not work

Assume

$y_p = A_2 x^2 + A_1 x + A_0$ which is realistic

$y' = 2A_2 x + A_1$

$y'' = 2A_2$

So

$2A_2 + 2A_2 x + A_1 = B_2 x^2 + B_1 x + B_0$

So ~~$B_2 = 2$~~ $B_1 = 2A_2$

$B_0 = 2A_2 + A_1$

$B_2 = 0$

Theoretically you could solve for the B's and then you have the A's.

The other approach is that you just solve for the coefficients as a part of the larger solution

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It is time to start formulating the problem.
Take D=2

$D^2 + D =$ ~~ax^2+bx+c~~ $ax+b$ Roots are $0, -1$

So model is $y = C_1 + C_2e^{-x} + ax^2 + bx + C$
will be sufficient. This means that

$$y = C_1 + C_2e^{-x} + ax^2 + bx$$

or we could say

$$y = ax^2 + bx + C_2e^{-x} + C_1$$

or $y = C_2e^{-x} + ax^2 + bx + C_1$

4 Points are needed for unique solution

$$\begin{array}{c} x_1 \\ x_2 \\ x_3 \ldots \\ \end{array} \left[\begin{array}{cccc} e^{-x} & x^2 & x & 1 \\ & & & \\ & & & \\ & & & \end{array}\right] \begin{bmatrix} C_2 \\ a \\ b \\ C_1 \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \end{bmatrix}$$

let $f(x) = x^2 \cdot \sin(x) + 3.0$

	X	f(x)		Superb Results
	0	~~0~~	3.0	3.0
1	~~5~~ .5	~~3.017~~	3.017	3.02
2	~~10~~ 1.0	~~3.~~	3.140	3.13
3	~~15~~ 1.5		3.471	3.48
4	~~20~~ 2.0		4.116	4.11

$V + B\Delta = f$
$V = f - B\Delta$

$C_1 = -.583$
$C_2 = .161$
$a = -.508$
$b = 3.583$

A superb solution has been achieved with

$$y = C_1 + C_2e^{-x} + ax^2 + bx$$

I modeled $x^2 \cdot \sin(x) + 3.0$

Now lets go to D^3.

$D^3+D^2+D = ax^2+bx+c$

(find y_h)   (this is y_p form)

Roots are 0, $-.5+\frac{i\sqrt{3}}{2}$, $-.5-\frac{i\sqrt{3}}{2}$

$$y = C_1 + C_2 e^{-.5x}\cos\left(\frac{\sqrt{3}}{2}x\right) + C_3 e^{-.5x}\sin\left(\frac{\sqrt{3}}{2}x\right) + ax^2 + bx$$

5 unknowns, use 6 pts

$$\begin{array}{c|c} X_0 & \\ X_1 & \\ X_2 & \end{array} \begin{bmatrix} 1 & e^{-.5x}\cos\left(\frac{\sqrt{3}}{2}x\right) & e^{-.5x}\sin\left(\frac{\sqrt{3}}{2}x\right) & x^2 & x \\ \vdots & & & & \\ \vdots & & & & \end{bmatrix} \begin{bmatrix} C_1 \\ C_2 \\ C_3 \\ a \\ b \end{bmatrix} = \begin{bmatrix} f \\ \\ \\ \end{bmatrix}$$

X_0	y
0	0
1	2
2	5
3	7
4	4
5	2
~~6~~	~~2~~

You really do have an amazing solution here.

I have done another version w/ ~~6~~ 7 measurements and 5 unknowns

Very good work.

Now lets set up a 4th order.

$D^4+D^3+D^2+0 = ax^2+bx+c$

Roots are $0, -1, i\ -i$

so

$y = C_1 + C_2 e^{-x} + C_3 e^{0\cdot x}\cos(x) + C_4 e^{0\cdot x}\sin(x) + ax^2 + bx$

or

$y = C_1 + C_2 e^{-x} + C_3\cos(x) + C_4\sin(x) + ax^2 + bx$

6 unknowns.

$$\begin{array}{c} x \\ 0 \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \end{array} \begin{bmatrix} 1 & e^{-x} & \cos(x) & \sin(x) & x^2 & x \\ \vdots & & & & & \\ & & & & & \end{bmatrix} \begin{bmatrix} C_1 \\ C_2 \\ C_3 \\ C_4 \\ a \\ b \end{bmatrix} = \begin{array}{c} f \\ \begin{bmatrix} 0 \\ 2 \\ 5 \\ 7 \\ 4 \\ 2 \\ 2 \end{bmatrix} \end{array}$$

Another excellent solution.

We may have predictive capability here...

$x=7$, $f(x) \cong 6.5$

$x=8$ $f(x) = 12.8$ fascinating.

I have a model that is potentially very valuable here.

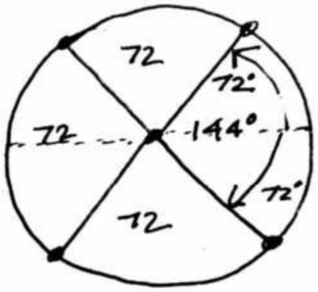
$D^5 + D^4 + D^3 + D^2 + D = ax^2 + bx + c$

Roots are $-.81 - .59i$, $-.81 + .59i$

$.31 - .95i$, $.31 + .95i$

0

So what is the pattern of the roots?



$3(72) + 144 = 360°$

$\frac{360}{5} = 72$

$\cos 72° = .31$ $\quad = .31 \pm .95i$

$\sin 72° = .95$

$\cos 144° = -.81$ $\quad = -.81 \pm .59i$

$\sin 144° = .59$

So the method is:

$\begin{matrix}\cos \\ \sin\end{matrix}\left(\frac{360}{n}\right) + \frac{360}{n}$

$\cos\left(\frac{K \cdot 360}{n}\right)$ $\quad K =$ [illegible] $1 \ldots \frac{n-1}{2}$

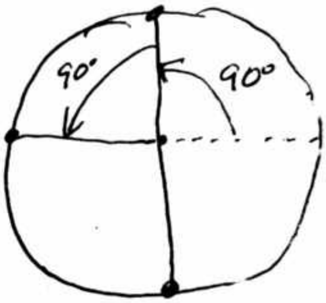
$\pm \sin\left(\frac{K \cdot 360}{n}\right)$

and 0.

What happens with D^4

$D^4 + D^3 + D^2 + D = ax^2 + bx + c$

Roots are 0, −1, i, −i



$n = 4$

$\frac{360}{4} = 90^\circ$

k=1 $\cos \frac{360}{4} = \cos 90^\circ = 0$

$\pm \sin 90 = (+1)i$ $\quad 0 + i$

$(-1)i$ $\quad 0 - i$

k=2 $\cos 2 \cdot \left(\frac{360}{4}\right) = -1$ leads to $-1 + 0i$

$-1 - 0i$

$\sin \left(\frac{2 \cdot 360}{4}\right) = \pm 0$

and this would be a repeat. How would you know this?

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CAD 2Hr Chart
Predict 0.2 Days (5HR)
Limit Time 12 HRS

It would be helpful if Math Studio can solve these scenarios.

Mathsoft on PC did solve it easily.

actual

Daily Intervals

0	12621	
1	12415	
2	12530	
3	12431	
4	12532	
5	12512	
6	12464	
6.2	12390	12583

Next Strategy
1. Pick direction
2. Choose S&R
Δ= 0.2 Days

Δ= 3.8!

Bias is up.
Two trades in place.
12hrs.

4	0	12424
5	1	12555
6	2	12440
8	3	12540
9	4	12513
10	5	12462
11	6	12580
	6.2	~~12680~~ 12650

~~Δ=46~~ σ = 3.8!

You have basically solved the Ultimate differential equation.

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AUD 10 MIN CHART
Predict 1 HR Limit Time 2HRS

AUD 7pts 10 min Chart

2hr Intervals

0	7779
2	7760
4	7734
6	7737
8	7717
10	7709
~~1100~~ 11.0	7707
~~11.5~~	
predict 12.0	7716

σ = 2.4 (3.3%)

Δ = 1 HR

Profit = 40
Stop = 25
Limit Time Interval = 2hrs

Always Consider
Supply & Demand

Supply & Demand Levels
are over interval of data being used.

EUR 10min

0	1318
2	1312
4	1307
6	1307
8	1293
10	1294
~~1115~~ 11.25	1287
12.5	× 1285

σ = 2.2 (7%)

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I believe that you have something monumental here.

You can make ST predictions @ any interval that you want.

Δ

2hrs Limit time = 2hrs perfect 10 min Chart

1 day Limit time 12hrs perfect 2 hr Chart

You can have multiple & staggered trades operative.
You can have unevenly spaced data!

3 Simultaneous Trades operative is very reasonable.

CAD : 12HRS limit
AUD & EUR : 2HRS limit

Your error rate on function fitting is on the order of 3-<u>10%</u>. Superb.

[redacted]

The probability model is:

$$P_r\% = \left(\frac{200}{\pi}\right)\tan^{-1}\left(\frac{\text{Interest Rate } C}{\cancel{\text{[illegible]}}} \cdot \text{Interest Rate}\right).$$

What is C?

$$C = \left(\frac{1}{\text{Range}}\right)\tan\left(\frac{\overset{9\,05\%}{P_r}\cdot\pi}{200}\right)$$

Spreadsheet Example:

$$C = \frac{1}{\text{Range}} * \tan\left(\left(\frac{\text{Range } P_r * \pi}{200}\right)\right)$$

decimal form

$$P_r = \frac{\left(\left(\frac{200}{\pi}\right) * \text{TAN}^{-1}(C \cdot X)\right)}{100}$$

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EUR 10 min		10 min		10 min
	EUR	AUD		CAD
0	1313	7654		2638
2	1334	7671		2587
4	1338	7691		2561
6	1334	7679		2555
8	1380	7705		2474
10	1405	7783		2458
11	1389	7742	11.25	2490
σ=2	1388	σ= 11 7732	σ=.5	2491

Acetone is highly absorbant in the UV spectrum.
Not @ all useful
Methyl Ethyl Ketone looks possible.
Alcohol is superb
Xylene looks moderately poor but not
as bad as acetone.

Feb 12 2015 Page 78

Something very strange w/ the alcohol emulsion test.
One worked, one did not?
Isoprop 70% — 90%
Water Mix?
Centrifuging?
Iodine – Pink

Method:

1. 1-2 ml of lipids
2. 23 ml of H_2O
3. 1-2 ml of 70% Walgreens Isopropanol
4. Shake
5. Centrifuge
6. Add Iodine (several drips)
7. Shake
8. Pink forms on upper layer!

The jar of Isoprop produced no reaction?
Actually there is red in all cases
Centrifuge reveals it.

Feb 13 2015 Page 79

Introductory lipid COB analysis is taking place
We learn that

1. It reacts strongly w/ iodine & also to some degree w/ saffranin. Iodine reacts strongly with double bonds.

2. Petroleum is not a lipid. Lipids are of biological origin. Fats generally have a "glycerine back bone". Petroleum is a mineral oil. Petroleum has no glycerine back bone.

Lipids are usually edible

3. pH Comes in @ about 7.4.

4. Does it burn?
   Yes, it is quite flammable.
   esp. w/ a wick

Suspect:
Triglycerides
(fatty acids attached to a glycerol molecule)
unsaturated

5. Refractive index? 1.488 This is very high.
Whole oil is 1.4760 ↑ Concentrated
X = 1.487
Second Measurement, Separate Sample 1.486
Cod Liver Oil R.I ≥ 1.4790, also 1.480-1.483

Comparison to Cod Liver Oil & Fish Oil:

1. Neither one is giving a iodine reaction.

2. Need flame test & Index of Refraction.
Cod Liver Oil fails the flame test.
3. Fish oil also fails the flame test.
4. Cod Liver Oil 1.478
Measured Index of Refraction
Stated Measurements are 1.479 to 1.483
Fish Oil measures in @ 1.480

Look @ solubility as a function of polarity!
This is important.

Polar Lipids are glycolipids & phospholipids)
(more soluble in polar solvents such as alcohol)

Non polar lipids such as triacylglycerols
are more soluble in non polar solvents such
as hexane.

So we know it is
1. a non polar lipid
2. a high refractive index
3. reacts with iodine - double or triple bonds
4. flammable - high carbon content
5. pH 7.4

6. Gram negative Stain

Highly polar indicates ?

Cod Liver oil is polar (dissolves in xylene
more readily than alcohol)
so it has ~~that~~ similarity along w/
index of refraction.

Fish Oil same thing. ~~These~~ They're
polar also.

$$H - C = C - H + Br - Br \Rightarrow H - Br - C - C - H - Br$$

Saturated fats are solid @ room temperature.
Saturated fats have no double bonds.

Unsaturated fats are liquid @ room temperature
Unsaturated fats have double bonds (creates gaps)

Oily Fish contain unsaturated fats.

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Our hypothesis is thus far.

But saturated fats are usually non polar? So what does this mean?

1. Non polar

2. Unsaturated (possibly highly poly unsaturated) due to reaction w/ Iodine

3. High refraction index, similar to many fish oils & whale oil (omega-3)
   High refraction index correlates with
   EPA
   ~~DHA~~ DHA !
   & total poly unsaturated fatty acids.

4. It is combustible - this indicates a high carbon content? whale oil?

5. pH is 7.4

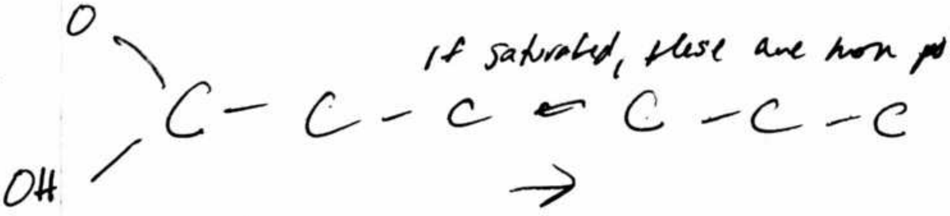
6. The fact that it reacts with a haligen so readily may not be encouraging.

We know the lipid dissolves readily in a non polar solvent (xylene). This suggests a longer hydrocarbon chain.

Polarity would seem to relate primarily to the length of the hydrocarbon chain. Saturation and liquid character) seems to relate primarily to the no. of available double bonds, regardless of how long the hydrocarbon chain is.

this is polar

If saturated, these are non polar.



The length of the chain would seem to be the primary indicator of polarity or non polarity.

The fact that we have a high refraction index indicates long fatty acid chains (eg DPA & EPA) and poly unsaturated fats

The indicates long chains w/ more numerous double or triple bonds.

Double bonds cause a bend in the alignment.

EPA is a 20 carbon chain w/ 5 double bonds. Yes it is definitely bent!

The long chain must be dominating non-polarity even though CIS bonds tend to increase polarity since they are on one side

DHA is a 22 carbon chain w/ 6 CIS double bonds. It is also highly bent.

We have 3 new oils to test

Linseed
Hemp
Flax

IOR
Flame Test
Iodine Test - Alcohol

Linseed IOR 1.479 Stated as 1.479 perfect.
Fails the Flame Test

Hemp 1.477 Cold Pressed Oil Stated @ 1.477 Perfect
159 is Iodine Value

Flax 1.479
175 Iodine Value
So this is <u>the same</u>

you have a good equation

Iodine Value = 4765.6 (IOR) - 6875.6
$n = 13$
$r = .92$
$r^2 = .849$

CBD Lipid IOR = 1.488 Iodine Value $\cong$ 215.6 $\cong$ 216

CDB

The method for lipid - iodine reactions is

1/3 CDB lipids
1/3 70% Isopropyl
1/3 water

~~Shake the~~ Mix thoroughly.
Centrifuge
Blank w/ lipids CDB
After settling a centrifuge the solution
should be clear and red.

Can we run a least square on the Classpad?

$$\begin{array}{cc} x_1 & \\ x_2 & \end{array}\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 1 \\ 3 \end{bmatrix}$$

$$(B^t B)^{-1} (B^t f)$$

2,3 3,2 = 2,2

C = 2,2 this is correct

$$\overset{3\times 2}{\begin{bmatrix} 1 & \exp(-1) \\ 1 & \exp(-3 \end{bmatrix}} = \begin{bmatrix} 1 & \exp(-a) \\ 1 & \exp(-b \end{bmatrix} = B$$

2 values for x=3

$$\begin{matrix} 1 & \exp(-3) \\ \vdots & \vdots \end{matrix}$$

B is now defined

Can we now go after $(B^t B)^{-1} = C$?

Looks like we have it. $(\mathrm{trn}(B) * B)^{-1} \Rightarrow C$ OK

Now define f. $\begin{bmatrix} 4 \\ 6 \\ 7 \end{bmatrix} = f$ Now ~~$C \cdot f$~~ $B^t f \Rightarrow D$ OK

~~$C \cdot (B^t f)$~~

Then $C * D = E$ E is the unknowns! OK!

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Least Squares on Class pad
Has Been accomplished.

1. Define "x" values

i.e.

$$\begin{array}{c} x_1 \\ x_2 \\ \vdots \end{array} \begin{bmatrix} 1 \\ 3 \\ \vdots \end{bmatrix} \Rightarrow \begin{bmatrix} a \\ b \\ \vdots \end{bmatrix}$$

2. Next setup B matrix

$$\begin{bmatrix} 1 & \exp(-a) \\ 1 & \exp(-b) \\ 1 & \exp(-b) \\ \vdots & \vdots \end{bmatrix} \Rightarrow B$$

redundant
x values
are needed.
This is Ok.

3. now solve for $(B^t B)^{-1}$
as
$(trn(B) * B)^{-1} \Rightarrow C$

4. Now define f :

$$\begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ \vdots \end{bmatrix} \Rightarrow f$$

5. Now form $B^t f$ as "D"
$trn(B) * f \Rightarrow D$

6. Now go after unknowns Δ, Call it E
$C * D \Rightarrow E$ (these are the unknowns.!)

Good work

Sipposedly you can redefine the X_i & the f_i and come up with a new solution. Lets try it.

X_i: Current matrices are:

$$\begin{matrix} X_1 \\ X_2 \end{matrix} \begin{bmatrix} 1 \\ 3 \end{bmatrix} \Rrightarrow \begin{bmatrix} a \\ b \end{bmatrix}$$

(lower case)
$(n \times 1)$

$$\begin{bmatrix} 1 & e^{-a} \\ 1 & e^{-b} \\ 1 & e^{-b} \end{bmatrix} \Rrightarrow \underset{(3,2)}{B}$$

$B\Delta = f$

$$\Big(\underset{(2,3)}{trn(B)} * \underset{(3,2)}{B}\Big)^{-1} \Rrightarrow \underset{(2,2)}{C}$$

$(B^tB)^{-1}$

$$\begin{bmatrix} 4 \\ 6 \\ 7 \end{bmatrix} \Rrightarrow f$$ (lower case)

f

$$\Delta = \begin{bmatrix} 6.891 \\ 2.119 \end{bmatrix}$$

$trn(B) * f \Rrightarrow D$

$B^t f$

$C * D \Rrightarrow E$

$(B^tB)^{-1}(B^tf) = \Delta$

unknowns!

Truth is, you would likely only change the values for f.

Changed f to $\begin{bmatrix} 4 \\ 6 \\ 8 \end{bmatrix}$ and it recomputed all automatically! to $\Delta = \begin{bmatrix} 7.470 \\ -9.431 \end{bmatrix}$

It worked!

Now we just scale up the problem.

Very Clever Work Here.

What if I want the V's. I have them.

$$V + B\Delta = f$$

$$V = f - B\Delta$$

or

$V = f - B \cdot E$ in our case.
So try:

$f - B \cdot E \Rrightarrow V$ and display residuals!

Yes, it gave me the results as

$$\begin{bmatrix} 0 \\ -1 \\ +1 \end{bmatrix}$$

This is great.
I have unknowns & V's.

This is really smooth. I change f and I get everything recalculated.

variables:	So matrices are:
a,b,c,d...	1. Assign x_i's to a,b,c, etc
B	2. B matrix Constructed
C	3. C matrix Computed $(B^tB)^{-1}$
f	4. f matrix assigned
D	5. D matrix Computed (B^tf)
E	6. E matrix Computed $(B^tB)^{-1}(B^tf) = C*D = \Delta$
V	7. V's Computed $f - B*E \Rrightarrow V$

Looking @ "eigenvibrations"

$my'' + ay' + by = 0$

$= m\lambda^2 + a\lambda + b = 0$ $\qquad$ $ax^2 + bx + c$

quadratic eq. $\qquad$ Period

$$\frac{-a \pm \sqrt{a^2 - 4mb}}{2m} \qquad 2\pi\sqrt{b/m - a^2/4m^2}$$

Interesting relationships going on here between eigenvalue & the period. p 327 Alexsandrov

$$\frac{-a}{2m} \pm \left(\frac{a^2 - 4mb}{2m}\right)^{1/2} \Rrightarrow \frac{a^2 - 4mb}{4m^2}$$

$$\boxed{= \frac{a^2}{4m^2} - \frac{b}{m}}$$

yes so

Eigenvalues $\qquad$ Not sure how this is done $\qquad$ Period

$$= \frac{-a}{2m} \pm \sqrt{\frac{a^2}{4m^2} - \frac{b}{m}} \Leftrightarrow 2\pi\sqrt{b/m - a^2/4m^2}$$

OK to here

Now is relationship between

$f \cdot \lambda \overset{?}{=} 1$ "cycle" if freq is 5 times per sec

or in this case $\qquad$ then $\lambda = 1/5$ $\qquad$ yes

$f \cdot \lambda = 2\pi$ radians

$$\frac{-a}{2m} + \left(\frac{a^2}{4m} \frac{-b}{m}\right)^{1/2} (x) = 2\pi$$

is for some reason the $-a/2m$ term not included?

$$\left(\frac{a^2}{4m} \frac{-b}{m}\right) x^2 \overset{?}{=} 4\pi^2$$

$$x^2 = \frac{4\pi^2}{\frac{a^2}{4m} \frac{-b}{m}}$$

$n=7$ Exponential Harmonics

$$\begin{bmatrix} X_0 \\ X_1 \\ X_2 \\ X_3 \\ X_4 \\ X_5 \\ X_6 \end{bmatrix} \quad 7\begin{bmatrix} 1 & e^{-X_0} & \cos & \overset{6}{\sin} & X_0^2 & X_0 \\ 1 & \vdots & & & & \\ 1 & & & & & \\ 1 & & & & & \\ 1 & & & & & \\ 1 & & & & & \\ 1 & e^{-x} & & & X_6^2 & X_6 \end{bmatrix} \begin{bmatrix} f_0 \\ f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \end{bmatrix}$$

$$(B^TB)^{-1} B^t f = \Delta = 6\times 1 \begin{bmatrix} \Delta_0 \\ \Delta_1 \\ \vdots \\ \Delta_6 \end{bmatrix}$$

$$(6,7)(7,6) \qquad (6,7)(7,1)$$

$$=(6,6) \qquad (6,1)$$

Now we take

$B\Delta = f$

and apply a new entry to the B matrix

this leads to a predicted f value @ X_6+1

Now we should have

$n=8$

$$\begin{bmatrix} X_0 \\ X_1 \\ X_2 \\ X_3 \\ X_4 \\ X_5 \\ X_6 \\ X_6+2 \end{bmatrix} \begin{bmatrix} 1 & e^{-X_0} & \cos & \sin & X_0^2 & X \\ 1 & & & & & \\ 1 & & & & & \\ 1 & & & & & \\ 1 & & & & & \\ 1 & & & & & \\ 1 & e^{-X_6} & & & X_6^2 & X_6 \\ 1 & e^{-(X_6+2)} & & & X_{6+2}^2 & X_{6+2} \end{bmatrix} \begin{bmatrix} f_0 \\ f_1 \\ \vdots \\ \\ \\ \\ f_6 \\ f_7 \end{bmatrix}$$

add $\overset{1}{2}$

n=1 For 12 hour prediction use 2 hr charts w/ daily values
n=1 For 2 hr prediction use 10 min chart w/ 2 h-values

Now we should get a different set of Δ?

n=1 Original Δ	Orig v's	n=8 Now Δ	Now v's
7.856E3	-.27	same? 7.84E3	Same -.6
40.523	2.595	108.1	except 5.7
11.268	-4.818	13.36	-7.7
-4.9	3.738	-4.50	1.5
1.235	-3.975	.97	-3.3
-19.214	5.195	-14.853	5.2
	-2.405		2.3
			-5.0

$v_7' \overset{\sim}{=} \emptyset$ Why?

Because you needed to add X_6+2 not X_6+1 !

OK, this looks very reasonable now.

AND examination

X	f	actual
2	7819	
4	7799	
6	7793	
8	7779	
10	7777	
12	7821	
13.75	7823	
14.75	7831	
15.75	7849	15: 7842

X = 7840 actual 7842!

this is about as perfect as you can get.

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Try a new setup on AUD Feb 22 2015

	AUD	CAD	EUR
4	7834	2443	1333
6	7845	2453	1309
8	7819	2551	1293
10	7829	2504	1361
12	7839	2521	1390
14	7841	2545	1375
15	7842	2534	1378
16	7861	2469	1409
17	7882	2465	1435
$\bar{x}$	7872	2442	1422

Set Trade - @ 7880. Good.

On any Chart, you will predict for a maximum of one interval.

eg Prediction Intervals:

40/25 10min ! Interval = 2 hrs (max prediction)

50/30 2hrs: Interval = 24 hrs (max prediction)

60/40 4 hrs: Interval = 48 hrs (max prediction

70/45 8hrs: Interval = 1 week (max prediction

Feb/23 2015

The probability function is:

$$\Delta X_i = \frac{1}{C} \tan\left(\frac{P_r \pi}{200}\right)$$

$$\text{Prob} = \cancel{\frac{200}{\pi} \tan^{-1}(C \cdot \Delta X)} = \frac{200}{\pi} \tan^{-1}(\Delta X \cdot c)$$

$$C = \frac{1}{\Delta X_i} \tan\left(\frac{P_r \pi}{200}\right)$$

Always err on the safe side w/ a margin of

0, 20, 50, 80, 100

Next, notice the highly correlated trades.
This is very dangerous.
You essentially have 3 trades of the same nature.
This is a recipe for disaster.

Ok, news should be @ 2 by default.
1 only if things are very quiet.
And watch for the 3's especially @ the right time of day.

Page
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10 min

2 HR

		CAD	EUR		CHF	AUD
0	10	~~1~~2428	1355	19	9404	7794
1	12	2428	1358	20	9576	7823
2	14	2424	1364	22	9373	7815
3	16	2435	1363	23	9442	7826
4	18	2438	1361	24	9493	7760
5	20	2436	1368	25	~~9492~~ 9480	7884
6	2200	2429	1371	26	9492	7856

Not usable.

News: No major news. Check this before prediction -

~~2586~~
2522

			7895 (6)
2435 (2)	1372 (2)	9584 (15)	~~7889~~ (4)
2424 (2)	1362 (2)	9446 (6)	~~7751~~ (16)
			7748 (18)

The two hour solution is completely out of sight.

You are trying to predict to the 20th which is impossible.

You should be using X + 0.5 X + 1.0

X + .25
X + 0.5

Predict less for more powerful dates.

No

2436	1372	9573 (13)	(3) 7883
2425	1362	9457 (4)	(15) 7761

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[redacted]

Mar 03 2015

The iodene complex is an interesting case.

Complex

Oklahoma

1. Olch

2-Cymes Morgellons

3. Environmental Law

Lancaster
Environmental Labs

3,4,1
Prox
1 m h

3,2,1
Strength

IR Prob Model

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~~3,2,1~~

CDB Lipids IR Spectrum

3	m	2	2900	alkane	C-H stretch	6✓
3	m	~~3~~2	2820	aldehyde	C-H stretch	6✓
3	S	3	1690-1700	unsat. ~~Unsaturated~~ Ketone	C=O stretch	9✓
1	(?) variable	2		alkene	could be CC stretch	2
2	S	3	1410	Phosphonic acid	P=O Stretch	6✓
2	m	2		amide	C-N Stretch	4✓
1	m	2		alkane	CH3	2✓
3	m-S	2.5	1210	Silane	Si-C Stretch	7.5✓
2	S	3	(1285-1110)	Ether	C-O-C Stretch	6✓
3	S	3		Phosphonate	P=O Stretch	9✓
3		3		Carboxylic acid	C-O Stretch	9✓
2		3		Ester	C-O-C Stretch	6✓
1		3		Sulfate		3
2		2		Phosphine		4

Infra Red Spectrum Model

IR Model Weight = Proximity Weight (3 to 1; Center, Edge, outside) * Strength Weight (3 to 1; S, m, weak) * Fingerprint Weight (1450-600) (2, 1; Fingerprint = 1)

3, 2, 1
Score

IR prob model

1450 to 600 is fingerprint region

Method of Analysis should be

Proximity

1. Weighting by intensity
2. Weighting by proximity to central location
3. A summation function

Summary Scores:

~~alkane: 6+2 = 8 no Competition~~

~~aldehyde 6 no Competition~~

Ranking by Scores:

Probability Table

		Weight of wavelength			
Phosphonate	9	1	9	90%	45%
Carboxylic Acid	9	1	9	90%	45%
Ketone	9	2	18	90%	90%
Alkane	$6^{(2)}+2^{(1)}=8$		14	80%	70%
→ Silane 7.5(i)			7.5		37%
Aldehyde	6	2	12		60%
Phosphonic Acid	6	1	6		30%
~~Ether~~	6	1	6		30%
Ester	6	1	6		30%
Amide	4	1	4		20%
Phosphine	4	1	4		20%
Sulfate	3	1	3		15%

$$C=\frac{1}{\Delta x_i}\tan\left(\frac{Pr\,\pi}{200}\right)$$

$$C=\frac{1}{\cancel{9}18}\tan\left(\frac{90\cdot\pi}{200}\right)=\cancel{.002742}\ \cancel{.0274}\ .00137$$

$$Pr=\frac{200}{\pi}\tan^{-1}(C\cdot\Delta x_i)$$

[redacted]

So the Final Probability Table is:

Ketones	90%
Alkanes	70%
Aldehyde	60%
Carboxylic ~~Aci~~ Acid	45%
Phosphonate	45%
Silane	37%
Phosphonic Acid	30%
~~Eth~~ Ether	30%
Ester	30%
Amide	20%
Phosphine	20%
Sulfate	15%

This was probably not a bad model.

Blood Pressure Data Mar 11 2018

	1A 1B	2A 2B	3A 3B	4A 4B
	[redacted]	[redacted]	[redacted]	[redacted]
	[redacted]	[redacted]	139 - 91	144 - 78
	119 - 81	139 - 74	135 - 91	132 - 70
	117 - 76	134 - 75	132 - 87	123 - 69
$\overline{X}$	122.3 - 79.7	136.3 - 73.7	135.3 - 89.7	133.0 - 72.3
σ	6.18 - 2.62	2.05 - 1.25	2.87 - 1.89	8.60 - 4.03
$\Delta\overline{X}$			+13 +10	~0 ~0

Conclusions:

1A — 2A $p = .020$
1B — 2B $p = .023$

No significant difference between [redacted] & Walmart machines

3A - 4A $p = .68$
3B - 4B $p = .002$

[redacted] reads 10 high on both numbers on our machine

1A - 3A $p = .03$
1B - 3B $p = .006$

[redacted] is in agreement with [redacted] Wal Mart

2A - 4A $p = .55$
2B - 4B $p = .60$

Our machine makes a difference if an extra shirt is on or not. Take it off.

3,2,1 Prox 1mich

3,2,1 Strength

IR Prob Model

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~~3,2,1~~

CDB Lipids IR Spectrum

3	m	2	2900	Alkane	C-H stretch	6✓
3	m	2	2820	Aldehyde	C-H Stretch	6✓
3	S	3	1690-1700	~~Unsaturated~~ unsat. Ketone	C=O Stretch	9✓
1	(?) variable	2		Alkene	could be CC stretch	2
2	S	3	1410	Phosphonic acid	P=O Stretch	6✓
2	m	2		Amide	C-N Stretch	4✓
1	m	2		Alkane	CH3	2✓
3	m-S	2.5	1270	Silane	Si-C Stretch	7.5✓
2	S	3	(1285-1110)	Ether	C-O-C Stretch	6✓
3	;	3		Phosphonate	P=O Stretch	9✓
3		3		Carboxylic Acid	C-O Stretch	9✓
2		3		Ester	C-O-C Stretch	6✓
1		3		Sulfate		3
2		2		Phosphine		4

Infra Red Spectrum Model

IR Model Weight = Proximity Weight (3 to 1; Center, Edge, outside) * Strength Weight (3 to 1; S, m, weak) * Fingerprint Weight (1400-600) (2, 1; Fingerprint = 1)

Hydrogen - Carbon Combustion Analysis

Apr 02 2015

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There is more than one way of getting a molecular formula before modern instrumentation came into being.

Here is a process of combustion that was used. So it was not always so advanced.

H & C percentage composition by combustion apparatus is helpful helpful.

Pavia book! Spectroscopy on Tablet

Let's continue to improve & develop our model IR.

1. Location within band (central, edge, outside)
2. Width of band
3. Shape of band
4. Intensity of band
5. Group vs Fingerprint Section
6. Detailed analysis & understanding
7. Resonance, conjugation effects ?
8. Probability model applied.
9. The big picture always first.
10. Really really study, try to start developing structure.
11. Cross Correlation overlaps
12. Notice we multiplied weights, we did not add.
13. Try to calculate frequencies also.

Bond - wavenumber Relationships Developed

Lets start w/ omega-3 fish oil.

Our first major peaks are @

2980
2890 So this should be sp^3
2825

So let's see what this means by itself.

Lets work on the theoretical determination first.
Assume a carbon bond to begin with. (Stretching)

5, 10, or 15E5 dynes/cm
$K = $ ~~1, 2, or 3~~
usually 1 or 2

$$\bar{\nu} = 4.12\left(\frac{K}{\mu}\right)^{1/2}$$

$$\bar{\nu}^2 = 4.12^2\left(\frac{K}{\mu}\right)$$

$$\mu = \frac{4.12^2 \cdot K}{\bar{\nu}^2}$$

example

$K = 10E5$ dynes/cm
$\bar{\nu} = 1682\ \text{cm}^{-1}$
$\mu \overset{?}{=}$

$\mu = 6$

and

$$\frac{12(x)}{12+x} = 6 \quad \text{so} \quad 12x = 6(12+x)$$

$$12x = 72 + 6x$$

$$6x = 72 \qquad \underline{\underline{x = 12}}$$

So it is a C=C double bond!

Lets try ours:

C single

$$\mu = \frac{4.12^2(5E5)}{2980^2} = .96 \cong 1.0$$

$$\frac{12(x)}{12+x} = 0.96 \qquad 12x = (12+x).96$$

~~$11x = 12 \quad x =$~~

$$11.04x = 11.52 \qquad x = \underline{\underline{1.04}}$$

This is hydrogen
We are dealing w/ a C-H bond.

*

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Now, something has causes the bonds to shift. Why.
First, determine theoretical C-H bond.

$$\vec{V} = 4.12\left(\frac{5E5}{.923}\right)^{1/2} \qquad \frac{12(1)}{12+1} = .923$$

$$\vec{V} = \cancel{3.96} = 3032$$

Now, your bonds are all less than this. What does this mean? I anticipate saturation levels. Let us study.
So it has to be a modification of alkanes in terms of saturation.

There is a base table avaliable which is very handy.

OH	3400	$C \equiv C$	2150
N-H	3400	$C=O$	1715
CH	3000	$C=C$	1650
$C \equiv N$	2250	$C-O$	1100

and we can compare others.

Now back to alkanes. They yield 4 or more C-H stretching peaks. Bending peaks around 1475-1365 & we also have those on the omega-3. p31 Pavia

Bending occurs @ a much lower frequency than stretching.
Hybridization definitely affects the frequency.

$$sp > sp^2 > sp^3$$

$\equiv C-H$	$=C-H$	$-C-H$
3300	3100	2900

Now we likely have to sp^3 figured out for C-H @ 2900.

Now, what is happening @ 2980 & 2825?

1. Higher mass means lower frequency.
2. ~~Double bonds~~
   3 2 1 times
   Triple bonds > Double Bonds > Single Bonds
   higher frequency > lower frequency
   ie higher wavenumber > lower wavenumber.
3. Bending motions occur @ lower frequencies than stretching frequencies

3b. Resonance affects frequency - Resonance reduces K.

4. It seems for stretching motions
   Single bond = K ≅ 5E5 dynes/cm
   Double bond K ≅ 10E5 dynes/cm
   Triple bond K ≅ 15E5 dynes/cm

Now I think we can start to estimate bending K factors.

C-H ~~Bending~~ Stretching (Single bond) ~3000   C-H Bending (Single) ~1340

$\frac{1340}{3000} \cong 0.45$ So it is on the order of 0.5

But maybe 0.45 is close. This would mean that

	Stretch K	Bend K
Single Bond	5E5 dynes/cm	1.0E5
Double Bond	10E5	2.0E5
Triple Bond	15E5	3.0E5

This is our ~~[illegible]~~ own developed tables that can be used to estimate bending frequencies.

$V_{\substack{single\\stretch}} = 4.12\left(\frac{5E5}{\cancel{3000}\ u}\right)^{1/2} \cong 3000\ cm^{-1}$

$V_{\substack{single\\bend}} = 4.12\left(\frac{K^*}{u}\right)^{1/2} \cong 1340\ cm^{-1}$

So $3000 = 4.12\left(\frac{5E5}{u}\right)^{1/2} \Rightarrow 3000^2 = 4.12^2\left(\frac{5E5}{u}\right)$

$1340 = 4.12\left(\frac{K^*}{u}\right)^{1/2}$ $\quad 1340^2 = 4.12^2\left(\frac{K^*}{u}\right)$

$3000^2 u = 4.12^2\, 5E5$

$1340^2 u = 4.12^2 K^*$

$$\frac{K^* \cdot 4.12^2}{5E5 \quad 4.12^2} = \frac{1340^2 u}{3000^2 u} \Rightarrow K^* = \frac{1340^2}{3000^2} \cdot 5E5 = 0.1995 \cong \underline{\underline{0.2}}$$

So our idea is that bending K is approximately 0.2 of the stretching K.
A lower wavenumber means a lower frequency. This means the "spring" is stronger. (The spring is the bond).
So we can now estimate bending wavenumbers as well as stretching wavenumbers.

STRETCHING

So we have

$\bar{V} = 4.12\left(\frac{K_s}{U}\right)^{1/2}$

or

$U = \frac{4.12^2 \cdot K_s}{\bar{V}^2}$

$K_s = 5, 10, 15E5$ dynes/cm

BENDING

$\vec{V} = 4.12\left(\frac{K_b}{u}\right)^{1/2}$

or

$u = \frac{4.12^2 K_b}{V^2}$

$K_b = 1, 2, 3E5$ dynes/cm

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Testing this as a hypothesis, we have

2980
2890 This one has been assessed as C-H sp^3
2825

$2890(.2)^{1/2} = 1292$ We don't really see that one on the omega 3.

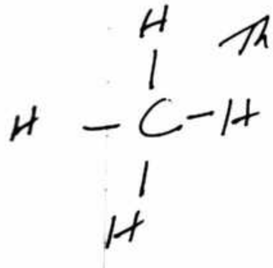
$2980(.2)^{1/2} = 1333$ We do see this.
$2825(.2)^{1/2} = 1265$ and we do not see this.
So this may be weaker, but still useful for comparison. It should probably be that you use the base values as you cannot get closer than that. eg
Single CH Stretch $3000(.2)^{1/2} = 1340$ & we do have this.
This would give us an ~~alkyne~~ alkane bend @ a reasonable location.

Notice that the base values only apply to the single "standard" bond, in the case of CH is must be a sp CH. Hybridization (ie saturation) in this case is an extremely important factor.

It appears to me that deviations from the base (theoretical values) will be one of your most important clues in interpreting the variation of bonds that are occurring & that will ultimately be of the greatest importance.

So let keep working on the omega 3 plot.
We have
2980
2890 - This is explained by sp³.   vs a theoretical base of 3032.
2825

This is methane.


$H-\overset{H}{\underset{H}{C}}-H$

3300	3100	2900
sp.	sp^2	sp^3

Now lets continue after the other two.
2980 & 2825 one higher, one lower.
2900. Methylene is CH_2 !!!! Watch your note.
Methyl is CH_3
Methane is CH_4
So what gives the slightly higher or lower peak?

It looks like the 2980 (2980 Noji) could be an asymmetric stretch of CH_3

Noji states that the 2890 is the stretch on a methane group w/ expected bending @ 1340.
Test this 2890(.45) = 1300 vs 1340. Only moderately ok.
Now, he says this is of no practical value but this is not necessarily true as it tells us that we have the hydrocarbon backbone of a fatty acid in place & I regard this as useful.

I also see us likely picking up a methyl group @ 2960 (Noji 2980) - this would be an asymmetric stretch and also potentially a symmetric stretch of a methylene group @ 2825 (Noji 2850).

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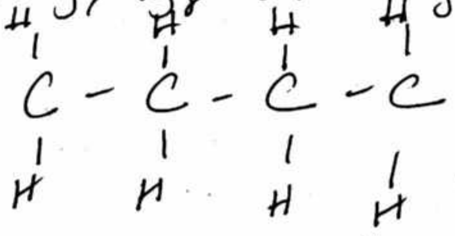
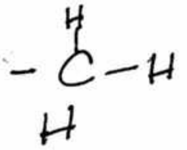
Now, notice Pavia says that we expect a methylene @ ~ 1465
(We look like we have it @ 1440)
He also says we have a methyl group @ 1375.
We have it.
He also says we could have a 4+ Chain of CH_2 @ 720
And indeed do we have a 690.
So this strongly suggests the omega 3 here..



$$\begin{array}{ccccccc} H & & H & & H & & H \\ | & & | & & | & & | \\ C & - & C & - & C & - & C \\ | & & | & & | & & | \\ H & & H & & H & & H \end{array}$$

It also should have a

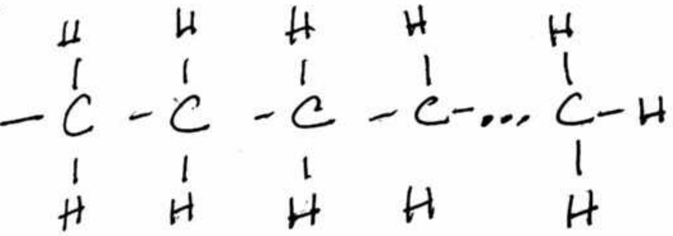


$$\begin{array}{c} H \\ -\overset{|}{\underset{|}{C}}-H \\ H \end{array}$$

a methyl

and we look also to have a CH_2
This is both from Pavia & Koji.
So this says

so something else should be attached to the open carbon.



$$\begin{array}{ccccccccccc} & H & & H & & H & & H & & H & \\ & | & & | & & | & & | & & | & \\ - & C & - & C & - & C & - & C & \cdots & C & -H \\ & | & & | & & | & & | & & | & \\ & H & & H & & H & & H & & H & \end{array}$$

Next we move to the peak @ ~ 1725.
What does this mo mean?
It positively seems to be a C=O bond.
What is this?

What is the base number? 1715

You are right on track.

P30 Pavia is <u>key</u>.

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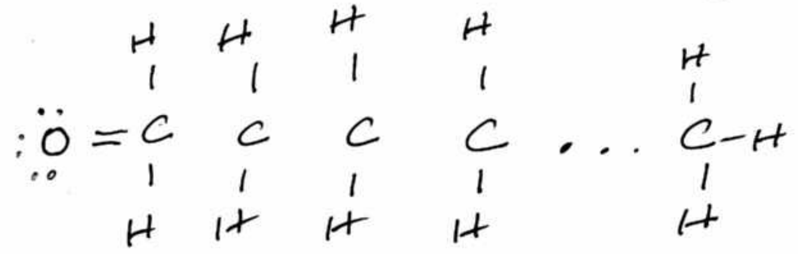
So now this indicates that we are dealing with the

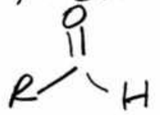


So what exactly is a $C=O$ by itself? Carbonyl Group

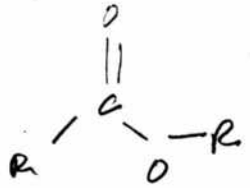
Aldehydes
Ketones
Carboxylic Acids
Esters

Oxygenated Functions

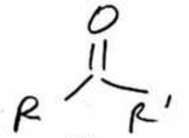
R-OH Alcohol



aldehyde

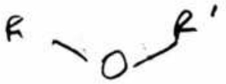


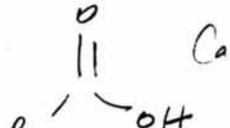
Ester



Ketone

Ok, Pavia places a big emphasis upon the Carbonyl group.
So yes, we have one.

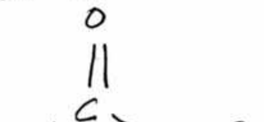




Carboxylic Acid

Now he is asking some questions.

OH present, no
NH present? Not that I can see
C-O present? Yes, quite possible. Strong absorptions near 1300-1000? Yes very strong @ 1160. So an ester is a real possibility. What is an ester?



Anhydrides? No
Aldehydes - Does not look like it. need 2850 & 2750. Do not have 2750.
Ketone. Everything else eliminated.

This now leads us to the prospect of.

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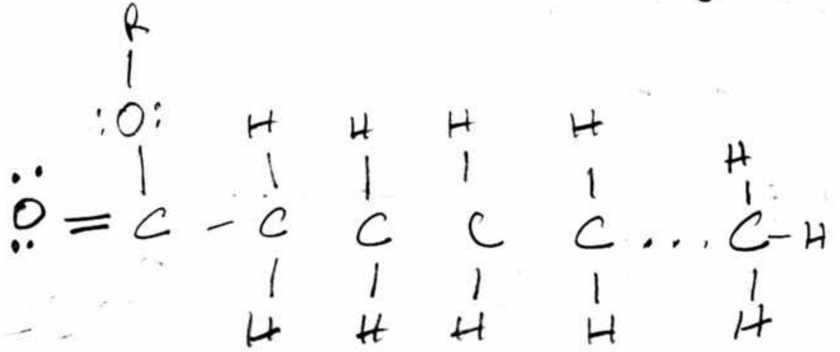
Now P51 Talks about the Carbonyl groups.



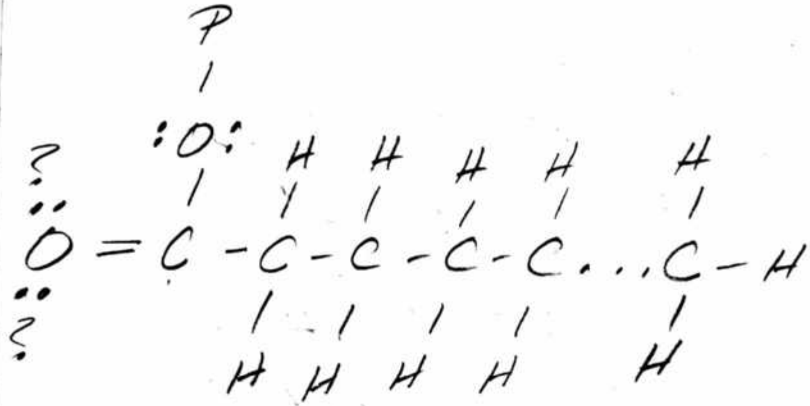
Ester base value is 1735. Looks to be on track
We can see there remain many opportunities for
Continued bonding. with the R group & the two O groups

Next we have activity @ ~1025
Phenols are an option here
Numerous opportunities @ 1025

	910 - 1040	Phosphonic Acid	P-O Stretch
	1030 - 1060	Sulfoxide	S=O Stretch
interesting	920 - 1090	Phosphoester	P-O-C out of phase stretch
	~~650~~		
	650 - 1000	alkene	C-H deformation
	1000 - 1110	Silane	Si-O-C Stretch
	1030 - 1160	alcohol	

Phosphoester is a real Candidate here.

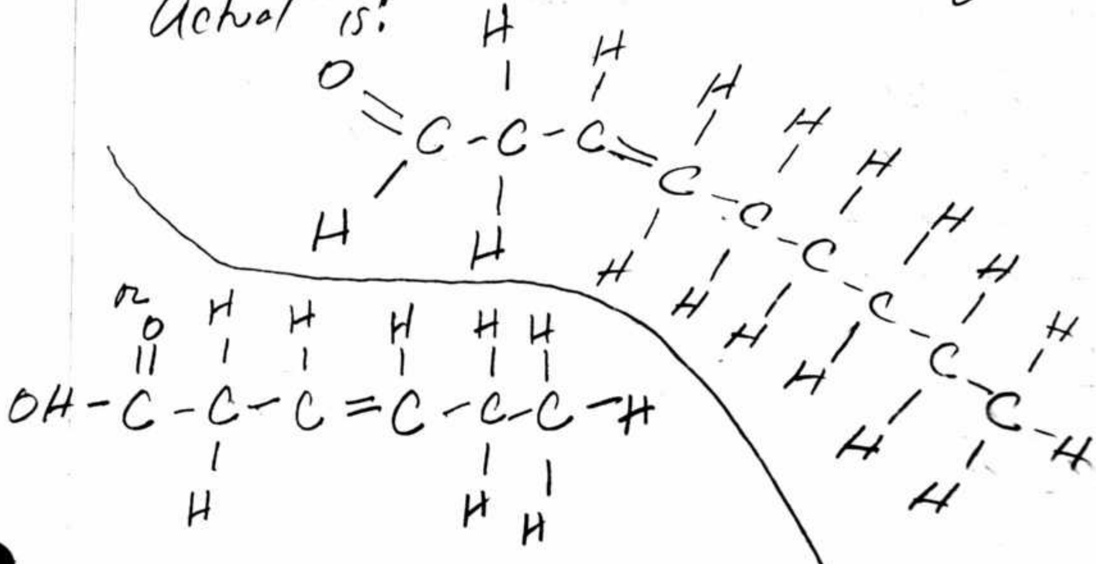
This leads to:



The ~~is~~ therefor your best estimate for the structure of an omega 3 fatty acid - fish oil.
How did we do?

So something happened here that we missed.
There is a C=C bond in the center
and an COOH group on the end that
made it an acid. How do we find these?

Actual is:



How did the errors happen?
Two of them C=C double bond & COOH

Let's look @ the C=C problem.
How did this happen?

From Pavia, the double C=C bond should have been uncovered between 1550 & 1650.
We do not have that in the slightest fashion.
So from Pavia I see no way of having it.

So this would be an ~~alkyne~~. alkene.

Now, from Chem Toolbox we definitely have an alkene from 1630 to 1680.
but recall we had ~ 1725.
This is a positive carbonyl group.

The 1000 - 650 "C-H" deformation" seems to be another possibility since we have a strong feature @ ≈ 690.

With Pavia we had a carbonyl group w/ no problem.

What happened is that we do not have the OH group. This is what caused the problem.
The OH is from 3250-3650.
We just don't have it.

Now Pavia has alcohols from 3400-2400
* and he says that it overlaps C-H
so this could be a factor.

There is saying to find an alcohol, if C=O is present, (which it is) we must consider the alcohol range all the way from 3400 - 2400 with an overlap w/ C-H which looks like it makes it undetectable.

However, if C=O is absent (which it is not!) then we would find an alcohol w/ broad absorption near 3300 - 3400. Which we do not have.

So carbonyls appear to be able to mask alcohols & therefore carboxylic acids. This is pretty important.

Maybe a better spectrum could help you further.

Look@ the massive drop taking place from 3600 - 3000 w/ CDB Lipids. It looks like a classic alcohol is taking place there.

It might be that the derivative is more useful than the peaks w/ our particular older instrument.
On the Omega 3 I just do not see the alcohol.

Note
*
This is unusual to say but in comparison to the few other highly unsaturated fatty acid spectra found the alcohol component does not always show up. How is that for a real trickster? How would you ever had made the determination of a fatty acid without it??

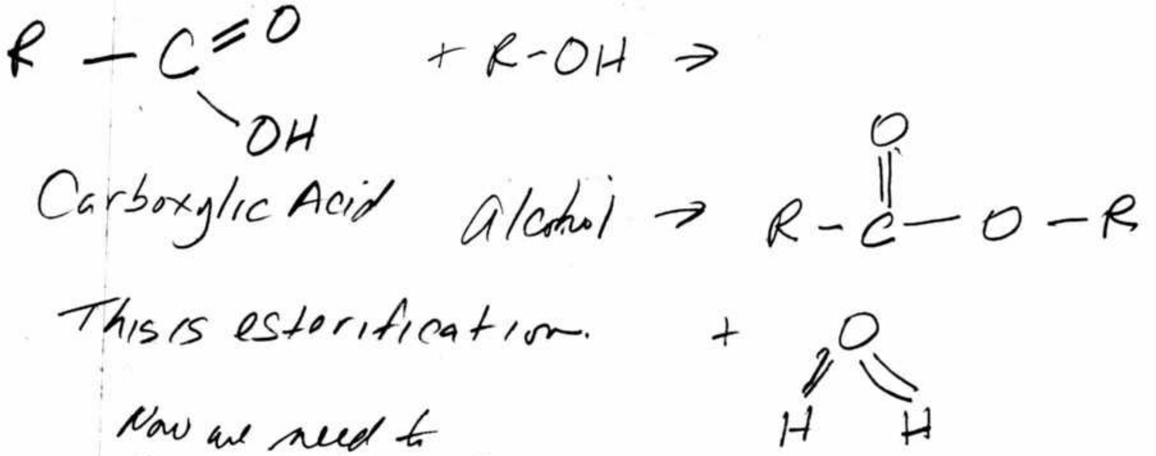
You may have found the answer to your dilemma! You may be right after all in your structure.

An ester is usually formed from an alcohol & an acid in the presence of a dehydrating agent.

Sound familiar, this is exactly what you are doing! Heating up a fatty acid!

So this actually is making rather perfect sense!

$RCO_2H + ROH \rightarrow RCO_2R + H_2O$

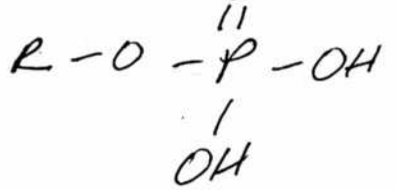


This is estorification.

Now we need to continue to work on the double C=C bond

Now remember the Company that showed a spectra that only showed the alcohol peak on a "old & used" oil

ester
There is an acid called a phosphoric acid ester.
It has the structure



$$R-O-\underset{\displaystyle OH}{\overset{\displaystyle O}{\overset{\|}{\underset{|}{P}}}}-OH$$

This is an "inorganic ester"

It says that esters can be derived from an inorganic acid and an alcohol

You may be on track a lot more than you thought you were.

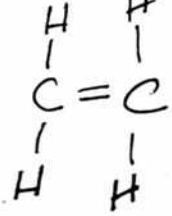
Now we can proceed to the CBB Lipids

CDB Lipids Examination

We have 2900 CH sp^3 ie CH_4
& 2830. CH_2 likely
We do not have 2980.

We also clearly have the Carbonyl group C=O
in this case, yes O-H is present.
This means we are dealing w/ an acid.

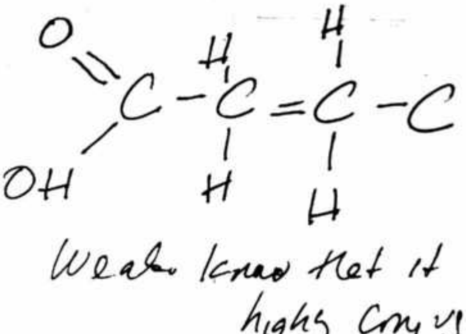
$$-C=C-$$



$$\underset{\displaystyle H}{\overset{\displaystyle H}{\overset{|}{\underset{|}{C}}}}=\underset{\displaystyle H}{\overset{\displaystyle H}{\overset{|}{\underset{|}{C}}}}$$

These would indeed be methylene groups

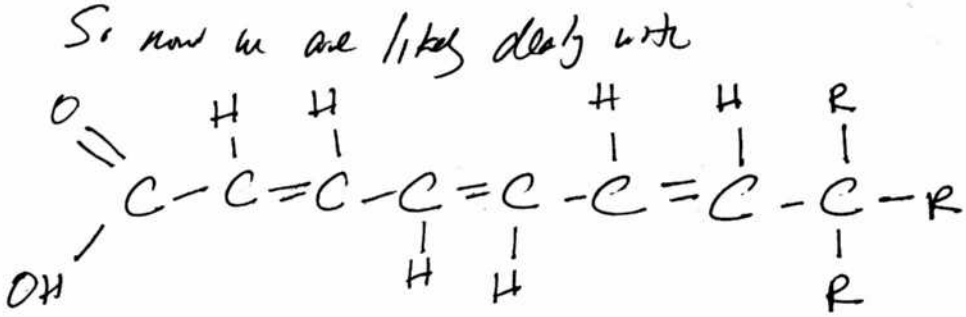
So already we have



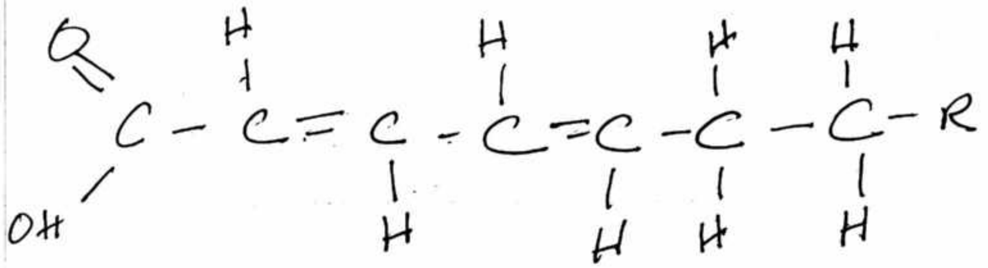
$$HO-\overset{\displaystyle O}{\overset{\|}{C}}-\underset{\displaystyle H}{\overset{\displaystyle H}{\overset{|}{\underset{|}{C}}}}=\underset{\displaystyle H}{\overset{\displaystyle H}{\overset{|}{\underset{|}{C}}}}-C$$

We also know that it is likely
highly conjugated.

So now we are likely dealing with

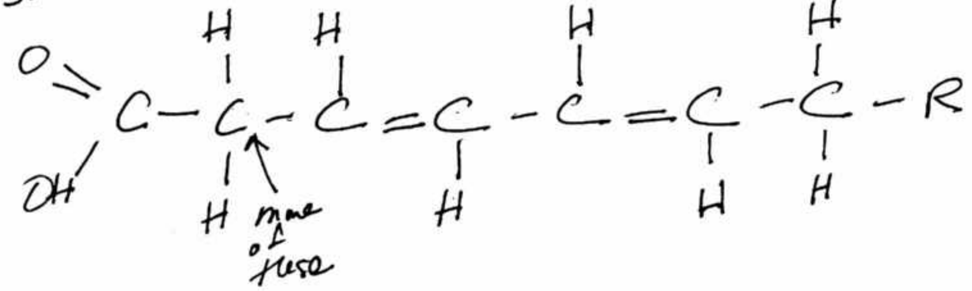


We have a 1410, & a 1270
We may have a 925 & a 720
but since we have a methylene structure
we should have

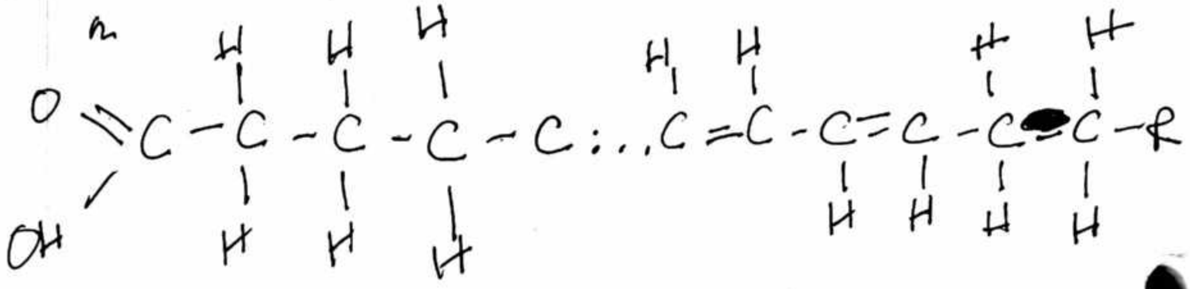


I believe we have the 4+ CH_2

So



or



So now what is 1270?

Candidates are

	Sulfate	S=O	1210 - 1260
	Silane	Si - C	~~1260~~ 1250-1280
	Ether	C-O-C	1110 - 1205
	Ester	C-O-C	1180 - 1290
	Phosphonate	P=O	1140 - 1320
*	Carboxylic Acid	C-O	1210 - 1320
	Phosphine	P-C	1250 - 1350

Any correlation w/ 925?

	Nitro	C-N	920 - 830
	Silane	Si-H	800 - 950
	Oxime	N-O	930 - 960
	Acid Halide	C-C=	920 - 965
	Phosphine	P-H	885 - 990
X	Alkene	C-H deformation	650 - 1000
	Phosphonic Acid	P-O	910 - 1040

Piavi's Correlation Chart is on p691
Page 30 is the overall View.
Let's carry on w/ the next spectra

We have lots of good sources now.
1. IR Pal if need be
2. LG Phone - Chem Tool Box - Not load one time
3. Noji - detailed
4. Piavi - the big picture p30
5. Piavi - Very detailed correlation chart p691
6. The test paper - Quickly & Correctly
We have worked on Omega 3 & CDB Lipids
and we have made good progress w/ both
Let's pick urine CEC next. 04-05-15

Very broad peak from 3600 - 3000
We also have strong peaks @ 3450, ~~3340~~ 3350 & 3200.
Lets work w/ these!
But the starting point is the Carbonyl.
Yes, we definitely have it 1660 - 1820.
We may also have more.
This means $C=O$ Now lets work with this.
Do we have OH? ~~I say yes 3400~~ Well this
is questionable. They say broad over 3400 - 2400
but I do not see it that wide.
Look @ the correct & quick paper for example.
Plot 377. The alcohol looks like an absolute given.
But notice that the "usual alkane sp^3 peaks just
below 3000" ARE NOT THERE!

This does say we have COOH
but what are 3450, 3350 & 3200 about.

So we are trying to determine, in addition to COOH
3450 3350 & 3200

We have 3420-3440 as amide. N-H stretch
This seems quite likely.

We also have 3340-3360 as an amide NH stretch.
Now we have increased probability.

We also have 3180-3200 as an amide. N-H stretch,

So the case looks very strong now as COOH NH
This was a great example.
We can develop a model for this. We need to know

1. Width of original measured band. } & How closely
2. Width of purported band } these correlate.
3. Our measurement of the center of our band & how it lies w.r.t. purported band.
4. The strength of the band, if possible.
5. Group in fingerprint region.
6. Base frequency of the bond?

Examples. We have very good results w/ the above.

Group Fingerprint	Width Measured	Center of Measured Band	Theoretical Width	Base Freq.	Prospect
Group	3600 - 3000	3330	3250 - 3650	3400	OH

meas 3600 ____ meas 3300 ____ meas 3000

75% 3650 ____ 3450 ____ 3250

	Left	Central ~~Right~~	Right ~~Central~~
	3600 - 3650	3300 - 3450	3000 - 3250 ~~3300~~ - 3450
	3650	3450	~~3450~~-3250
	= -1.4%	= 4.3%	= 7.7%
X-100	98.6	95.7	92.3

Carbonyl 1620 - 1820
You seem to have a good simple model here.

We have very good results so far

C=O 94.7%
OH 95.5%
Amide 99.4, 99.4, 99.7 so three times!
$\bar{X}$ = 99.5%

Lets look @ carbonyl peaks
1660 1640 - 1600 Amide
1620

Oxime	1680 - 1620	Keep these in mind. Solitary right now.
Amine	1650 - 1550	
Ketone	1650 - 1580	
Amide	1650 - 1530	
Arene	1630 - 1590	

OK, on we go to 1450:

Candidates: Meas Width. 1500 - 1400
Center 1450

1400 - 1450 is phosphine

One other @ 1140   1200 - 1000

So you may have good results, but how to weight them?

Weighting Factors:
1. Width of Band
2. Group & Fingerprint
3. No of entries.
4. absorbance value gives instensity.

~~(1-.03)~~ n 1-Abs

Our scores for urine are therefore: Ranked

Carbonyl	113.6	Amide ~~Alcohol~~	~~764.2~~ 950.8
Alcohol	764.2	Alcohol	764.2
Amide	950.8	Amine	737.0
Oxime	117.8	Ketone	139.0
Amine	737.0	Oxime	117.8
Ketone	139.0	Carbonyl	113.6
Arene	79.5	Arene	79.5
Phosphine	49.1	Phosphine	49.1
Alkane	19.6	Alkane	19.6

So we have made some progress, but there are still uncertainties.

Carbonyl is strong & obvious.

Ketones & Oximes are somewhat more questionable. Why do our results disfavor the strong Carbonyl?

1. First, we only have one entry.
2. The width should be weighted more.

Adjusted Score is now:

Alcohol	305696
Amine	81050
Amide	30510
Ketone	9729
~~Carbonyl~~	~~6818~~
Oxime	7070
Carbonyl	6818
Arene	3180
Phosphine	2457
Alkane	392

Maybe better
but why is the Carbonyl
still so low?
You are still missing
something.
I think it is the
absorbance.
(1-A)

or you could divide by absorbance

There is no alcohol!
It is a carboxylic acid!

Dividing by absorbance, the score is now

Alcohol	1,018,987
Amide	944,963
Amine	757,688
Carbonyl	227,250
Ketone	324,291
Oxime	235,653
Arene	
Phosphine	
Alkane	

Better

With width 3 cubed, score is now.

Alcohol ~~Carbonyl~~	40759	
Amide	11264	
Amine	9112	
Ketone	2270	
Oxime	1414	
Carbonyl	1364	Something still wrong here

I see. The given Carbonyl group is very limited.

OK. I see the problem.

I have found the answer and the error.

You do not have a Carbonyl and an alcohol. There is no such thing.

What you do have is a Carboxylic acid. Strong as can be.

The answer was found in the Spectra Quick & Correct Paper. — Carboxylic Acid Section Plot 437.

In the Carboxylic acid spectrum the OH peak is extremely broad and the Carbonyl is nice & sharp @ 1700.

One of the big lessons here is that the OH varies. If it is very broad it is a Carboxylic acid if it also combined with a sharp Carbonyl group. This is a huge lesson.

So your urine has a Strong Carboxylic acid in the sample.

Now you must adjust your model to pick up on this.

So the truth is the band went to 2200

Pavia was trying to tell us about the OH group!

Sometimes it is an alcohol, sometimes it is an acid!

!! The acid is a very broad OH combined with a carbonyl group

!! The alcohol has a broad but narrower OH with no carbonyl group

Your amides are still on track
and probably the amine as well.
But all bets are off in general.

Start Over! PAVIA was correct!!!

The acid showed up @ the top of his list. Pavia pegged the acid immediately. It took me about 3 hrs to get there.

He also pegged the amides immediately @ 3400. Even the double peak — (we have a triple peak)

Lets review how we came up w/ the amide.

Urine analysis

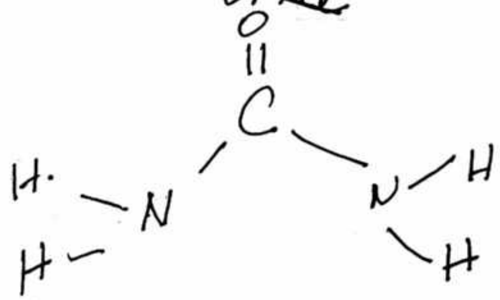
Cl
Na
K

Page 127

Amide
3480] triple peak
3380
3210

1640 also.

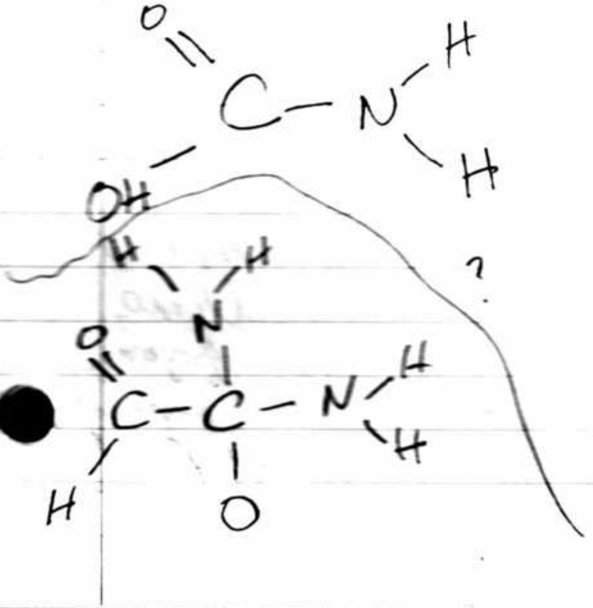
Urea
~~Urine~~



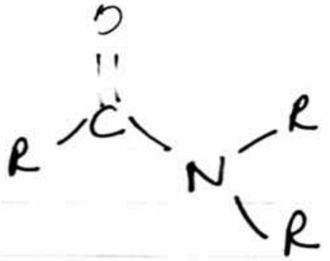
Also, it is not A that matters
It is ΔA

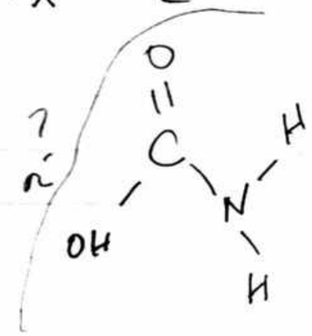
Now our ranking is

		~~log~~ ln	$\log_{10}$	
Alcohol	175754	12.1	OH	NH_2
Amine	1207	7.2	NH_2	NH
Carbonyl	545	6.3	C=O	N
Amide	99	4.6		
Phosphine	61	4.1		
Ketone	29	3.4		
Oxime	21	3.0		
Arene	10	2.3		
Alkane	10	2.3		



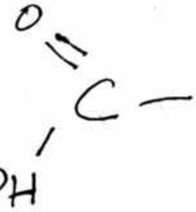
Amide
$R_n E(O)_x NR'_2$





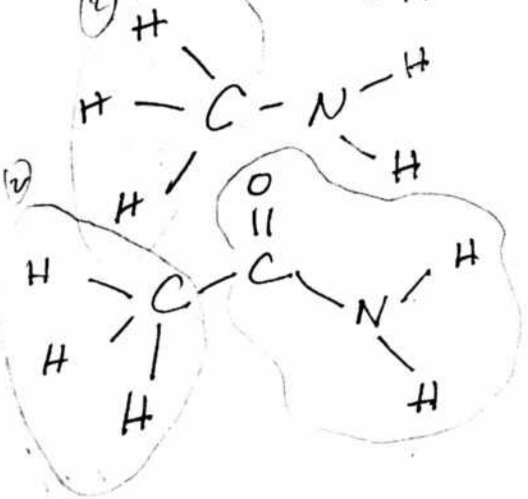
Urea Findings.

Carboxylic Acid

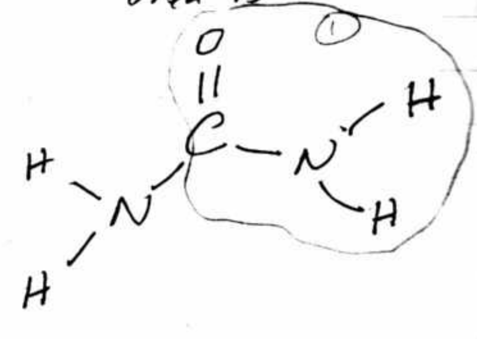


Amine

Amide



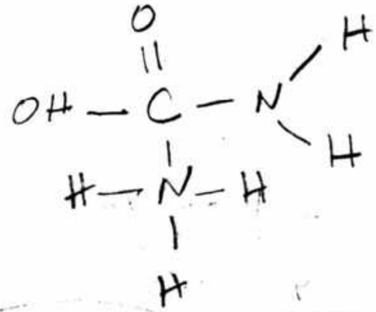
Urea is



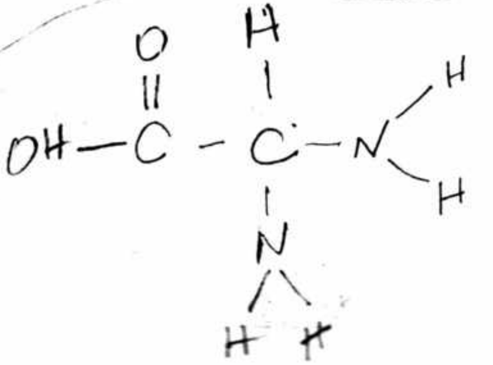
So we need to combine these in a minimalist fashion.

The right half to an amide is a perfect match to urea.

Nitrogen can apparently have 4 bonds at a time but then it has a charge



This looks good



Proposed Urine Organic Component w/ Acid

Apr 08 2015

I think that we are doing generally well and that we are making progress.

Let us go to the next one & we will revisit those previously done.

We have looked @

1. Omega 3 fatty Acids
2. CDB Lipids
3. Urine [redacted]

Let's look @ [redacted]

I am not sure if there is a carbonyl or not.
It is certainly not a sharp peak.
BP30 is the general view:
Carbonyl is 1660-1820
For both Carol & I the low point seems to be about 1500. This does not appear to be Carbonyl.
Let's continue w/ Pavia.
I say no carbonyl.
So assuming Carbonyl is absent, next question is do we have OH? Broad 3400-3300
But we have something huge 3600-2400.
This is what we saw is OH, but without C=O?
So this would indicate a definite alcohol
Notice Koji calls OH from 3200-2500
calls it chelation w/some extra bond
like C=O, NO_2

We have an interest[illegible]ter of an aromatic ring.
1600 - 1450.

Also an interesting C[illegible] of
"aromatic or vinyl CH to the left of 3000"
and aliphatic C-H to the right of 3000
We have both of these.

This suggests
1. OH
2. Aromatic ring
3. Aromatic or vinyl CH
4. Aliphatic CH.

Notice we also have strong absorbance near 600.

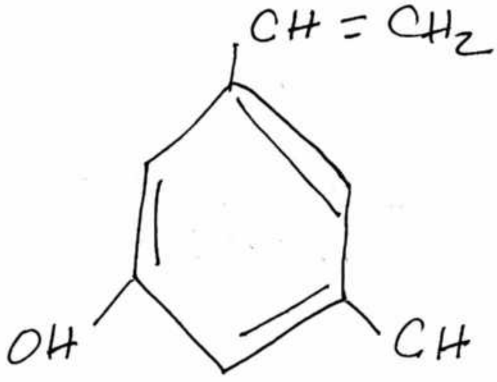
So 3250 Oxime fits.?
2920 Alkanes

Koji 3400-3200 "Polymeric OH"
Nothing else is really there? ...

What is a
Vinyl CH $-CH=CH_2$
Aromatic CH
Polymeric OH

Aromatic is a very strong candidate
1,3,5 substitution

Aromatic OK



Apr 10 2015 [redacted]

OK, lets go for the next one.
We learn so far that urine may have an acidic problem.
Blood may have an aromatic / phenol problem.
& that the COB lipid is indeed appears highly unsaturated.

Now lets go to the modified blood.
BUT before we do that, let's look at
[redacted] situation a little more closely
as [redacted] does show some increased activity.

[redacted] show activity @
~ 1465
~ 1400
1300
and ~~interestingly~~ enough we find these on the COB-blood combination but less clearly in [redacted] blood samples.
Ok, what do they mean?
From chemistry toolbox:

* 1465 (1450-1470) Alkane CH_2 deformation
* 1400 (1360-1400) Alkane CH_3 deformation

These are the simplest choices, there are others w/ wider bands involved!

* 1300 (1250-1350) Phosphine P-C
* (1300-1350) Sulfone S=O
(1320-1360) Nitro N=O stretch 2 bands, not likely

We see here that the alkanes CH_2 & CH_3 are reasonably consistent w/ the original analysis.

Now let's go to the CDB Blood Combo.
You pick up two very strong peaks here that are inherent w/in the CDB @
1640 vs No these do not match.
1520
Actually they do not really match anything from Chemistry Toolbox.

1520: (1480 – 1520) Arene
This set looks to be more difficult.

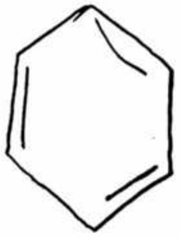
Now, let's make a run w/ IR Pal from the [redacted] Blood beginning.

Now, we have alcohol from 2400 to 3600 so this is missing the very broad peak from 2600 - 3600 which is what Pavia gave us right away.
What is happening here is that the alcohol is actually confined to the 3600 - 3300 range (Combined IR Pal w/ Pavia) assuming C=O is not present, which it does not appear to be.

The unusual situation is that our peak is exceptionally broad, on the order of 2400 - 3600 as expressed in Pavia Carbonyl section. But we do not have a Carbonyl.

Therefore, the interpretation become
that we have a combined peak
which is forming a broad major peak.
This makes sense. We have peaks @
3225
and 2920

that have combined into a single peak.
The 3225 is a phenol straight & clean
with IR Pal.



w/ OH
and H
where? are they
bonded.

Now the 2920 is a alkane. IR Pal. The
Carboxylic acid does not work.

Now Pavia is getting us to either an alcohol
or a phenol right away.
Pavia in step 4 gets us also immediately to an
aromatic ring.

Pavia is also suggesting that we have an
aromatic or vinyl CH
From Pavia the 2920 should be a CH sp3

However Pavia says we really need to be on the
lookout for
vinyl, aromatic, acetylenic or cyclopropyl
hydrogens to the left of 3000.

Page
135

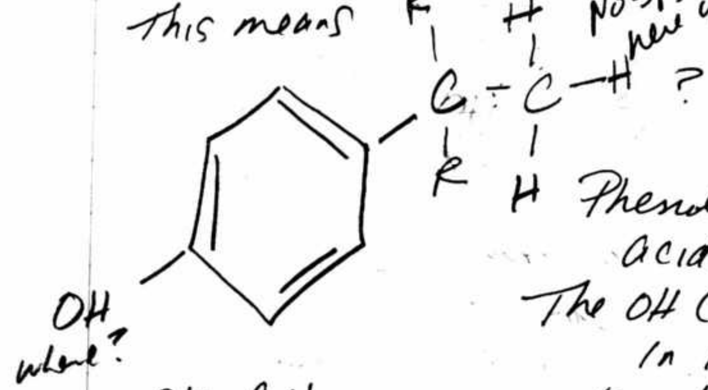
CEC Blood Analysis

This indicates that we very likely have

with OH & sp3 CH

it can always have more than one

This means



phenol will tell you where it is.

Phenols are much more acidic than alcohols.
The OH can and does vary in its location.

OK, let's move on. How do you get sp3 in a chain?

Phenol is produced naturally but it should be showing up in the urine. Concentration is 40 mg/liter.
But it poses serious problem. This is a whirlwind here.

Our next major peak is @ ~~1600~~ 1500. Pavia already set us up w/ a likely aromatic here.
Pavia aromatics are 1450 to 1600
IR Pal only gives us 1400 to 1500
Pavia once again comes out on top here.

EPA: Chronic exposure shows central nervous system, kidney, liver and cardiovascular effects.

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We now have fairly strong evidence that a phenol w/ aliphatic hydrocarbon structure exists w/in blood samples. This would appear to be unusual.

Shame

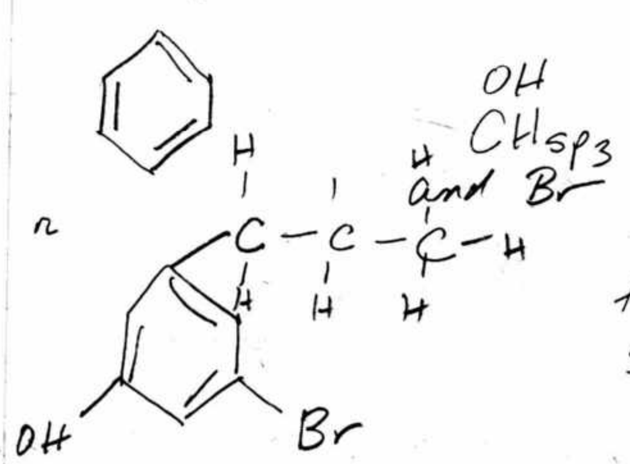
WIS

Give Plan Survey

Okay, serious business developing here. [redacted] blood sample activity from 1400 - 1100 is difficult to define. But I do have the strong decline which appears to go to and past the 600 level. Now, the aromatics appear to go to 690.

But what positively does go past 667 is the halogens of Bromide or Iodine.

This suggests now a structure of



this should be searched.

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The correlation chart & overview by Povia seems to be an excellent beginning in analyzing spectra. Then when you combine it w/ individual examination of each functional group it is even better.

[redacted] shows activity @
1465
1400
1300 - review this.
Now the toolbox indicated CH_2 alkane @ 1465 and a CH_3 alkane @ 1400. These coincide perfectly w/ your existing drawing. Can we find them in IR Pal also?

This also matches perfectly w/ Koji. He also suggests a CO along w/ CH_2

Remember Koji has a superb correlation table.

Now it could be a mistake to take the last peak @ 1300. The average looks closer to a 1280. The stronger choice in that case will be the phosphine P-C (1250-1350)
So @ this point this exists as a stray entry.
Lets look @ Koji. Koji shows
aromatic amines (1250 - 1360)
alcohols (1250 - 1500)
~~C=C-H 1400~~
Vinyl ethers or aromatic ethers (1200 - 1275)
CH_3 1145-1255

ketones, NO_2, aromatic N. oxides, P=O, POOH, C-F (1100 - 1400)

So what we see here is that the peak @ ~ 1280 holds numerous possibilities and many of them share overlaps w/ previously identified groups!

Now we can move to the CDB - blood mix. Lets take it from scratch

A huge broad peak @ 3600-2500.
Now we want to be careful here.
An alternative scenario from Pavia is that we consider a carbonyl. THIS IN NO WAY worked for solitary blood of both [redacted]
This means that even if we do have an alcohol there is no reason to think that we have an acid. It is interesting that Pavia does however associate an acid w/ a carbonyl & a wide broad peak from 2400-3400 exactly as we have as well as the overlap from C-H.
However the CARBONYL DOES NOT EXIST in the raw blood sample so that negates that approach.

BACK TO COB - Blood Mix

So now that return to blood - COB mix is there any reason to believe that we have induced a carbonyl. Not really.
What we see is activity @

2080 ~~2040~~ (possible?) $C \equiv C$ & lots of N activity
1635 Strong possibility of Nitrogen, or $C=C$
1525 Aromatics & Nitrogen activity

Kgji

1400 CH_2-CO, $C=C-H$, OH, SO_2
1300 C-F, SO_2, NO_2, aromatic amines, OH
1115 C-F, all over the place

Conclusion on CDB - Blood Mix

We are now seeing strong indications of a blood - CDB reaction upon mixing that is leading to nitrogen compounds forming, and even more so, likely that they are aromatic amines.

I have a new program on the tablet - IR Spec - and phone to test. It looks helpful. It does not have correlation. Let's test it - Use the Protein

OH broad? 3200-2400 broad?
2850. C-H alkone - exact match. methylene
2400 - vey small N-H amine
1420 C-H alkane, nitro
1330 N-O Nitro, aromatic
1130 C-N Amine
910 =C-H Alkene, Benzene ring
700 Alkyl Halide, Benzene ring, alkene

[redacted]

It might be a good idea to start all over again considering all sources ~~that~~ you have and how they can best be used together. IR Pal is also a very valuable tool that pulls in correlations. Takes more computing power but if you have it, go for it.

OK, lets go back to Omega 3.

2980 Something happens. Notice it is small.
From our master sheet we already know it is a single bond: C-N, CH, O-H or N-H
We also notice that it is a set. w/2900 & 2820.
It is also a sharp strong peak. Now remember Pavia always starts w/ the Carbonyl & that does seem like a very good idea.
Remember that we also know how to compute base values for various bonds & that we have a table. This is actually a lot of fun since it is based on theory & should eliminate many categories right away, at least w.r.t. stretching. We also even formed our own estimate on bending but this is more difficult. Pavia has the table on p30.
Hybridization (esp hydrocarbon) should not Cannot be ignored along w/ resonance.

P30 Strategy
P691 Full Corr Chart
P29 Corr Chart

P32 – 104

Page 141 *

~~P16~~ P15 – 31 is Foundational
You must know Ch 2 Pavia by heart
He is building a foundation here that
will serve you forever:

1. Base values
2. Hybridization
3. Resonance
4. Double, triple bonds (remember how it affects base values)
5. Stretching vs bending
6. Symmetric vs asymmetric.

This is a powerhouse.

So w/ Omega 3 we have
1725 Certainly looks like Carbonyl. This starts the whole flowchart.
IRSpec picks up the Carbonyl right away
looks exactly mid range. So this is a very strong Candidate.

Now, IR Pal misses this completely. He does not really even have carbonyl & he goes immediately to a very narrow range. This is not good @ all! He flies immediately to subgroups which is not helping matters. To miss the carbonyl is not @ all helpful here.

IR Explainer picks up the C=O stretch but also does not use the term Carbonyl and they also go immediately to subgroups. So we are clearly seeing variation.

Chemistry Toolbox also works.

So what you see is that
1. IRPal
2. IRExplainer
3. & ChemToolbox

] all of them pick up the assignment correctly.

It is in picking a "class" that the problem develops. You do not want a class yet, you only want the assignment or the groups. Any of the tools are ~~working~~ to pick up the assignment, the class will have to be reserved for late judgement.

Ok now we know from 4 different sources that we have a carbonyl, a C=O stretch assignment.

$\underset{\leftarrow}{C}=\underset{\rightarrow}{O}$

Now we can move on, and Pavia is always the best in terms of strategy.

So what is the base value? 1715

Not bad @ all. Is within error.

So we now have a carbonyl. Pavia:
He asks some questions.
1. No OH
2. Amines – NO (near 3400)

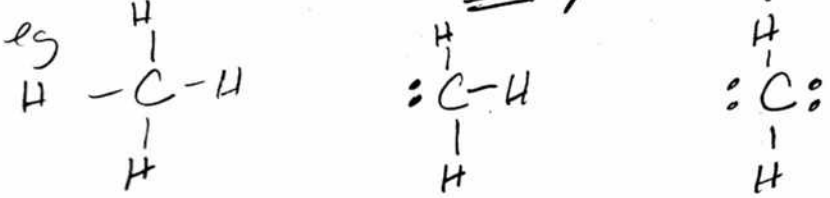
3. Ether.

Looks like we do have have this. This is a C-O-C Stretch.

Now we see that Pavia is skipping the ~~at~~ C-H absorptions @ 3000 but I really do not want to do this.
It provides the backbone.
I think the C-H bonds are very interesting, informative and important. They tell if something is a hydrocarbon ^ not.
So there is a difference between < 3000 + > 3000.
We are less than 3000.
2980
2900
2820

We know we are dealing w/ Sp³ here.
What Sp³ actually means is ~~so~~ that we have
No atoms attached + <u>lone</u> pairs = 4

eg



There are all SP_3

but we know the carbons still want to bond so they are not likely to stay lone pairs. We also see the rule (Org. Chem Workbook p14) says <u>atoms</u> - they do not have to be hydrogen!
Also the geometry is very important as they are <u>tetrahedral</u>.

Next Pavia tells us that we may have CH_2, which is methylene, bending @ 1465. We have it!

He also says that we may have CH_3, which is methyl, at 1375. We have it.

He also talks about having 4+ CH_2 groups in an open chain around 720. We seem likely to have it @ 690. So there is a lot of information coming in here from the C-H bond.

We now want to pin down
2980
2900
2820

more fully IR pal gives 2980 @ RCH_2CH_3

They give the same for 2900
Nothing given for 2820

2980 2900 IR Spec gives $=C-H_2$ alkene

This is getting confusing. Many types of ~~bonds~~ CH bonds.

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What we noticed from Pavia is that the hybridization discussion seemed to explain what we see perfectly.

We know from Pavia's hydridization discussion that we are dealing w/ sp^3 geometry @ ~ 2900. sp_3 means ~~single bonds~~. what it really means is atoms attached + lone pairs = 4.

What is the configuration of

≡C−H
↑
?

1. two atoms attached
2. no lone pairs

Sum = 2 means sp linear.

=C−H
↑
?

1. two atoms attached
2. one lone pair

Sum = 3 means sp_2 Trigonal Planar

−C−H
↗
?

1. ~~B~~. two atom attached
2. two lone pairs.

Sum = 4 means sp^3 tetrahedral

so sp_3 is referring to an atom

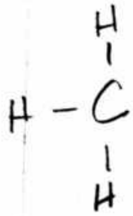
ie the geometry @ a particular atom, not @ a bond location.

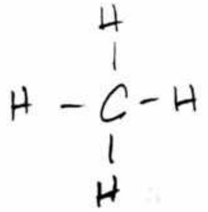
So we'll still have not figured out the nuances of

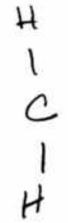
[illegible] 2980 CH_3 2960
[illegible] 2900 −C−H 2890 this is the backbone
[illegible] 2820 CH_2 most likely 2850

Chemistry Toolbox only picks up alkane here.

So what do we know so far?
We appear to have



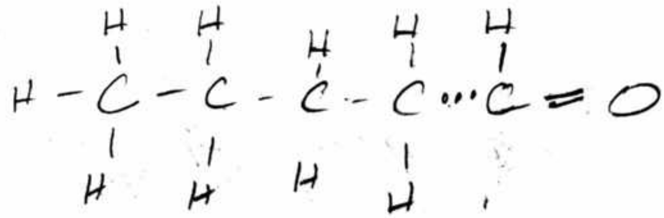




and C=O

and $n>4$

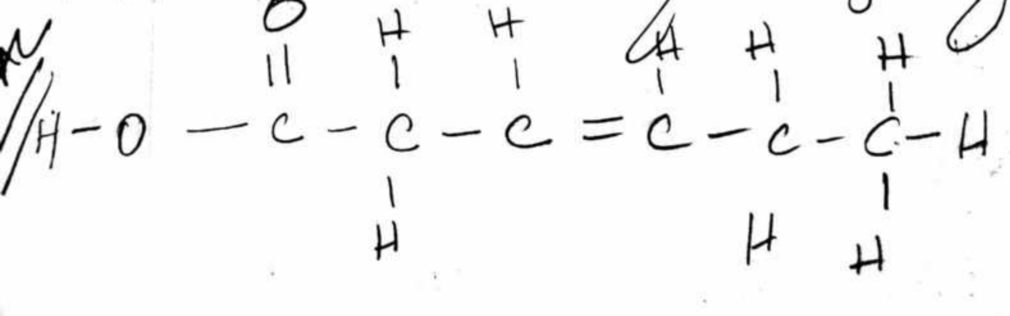
This suggests something to the effect of



This means the oil is unsaturated.
Now we would work on the fingerprint region.
~1150
~1020

IR Pal 1150 is full of options but
The ester looks like a possibility
RCOOR

The actual structure of an omega 3 fatty acid is



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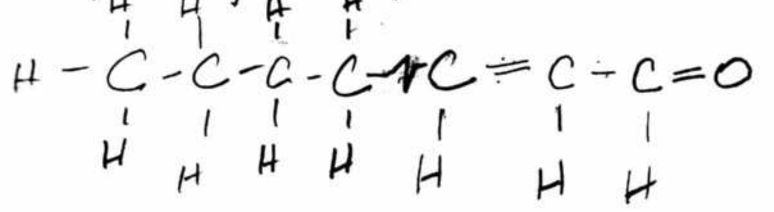
So what we have missed so far in the
C-O bond
The acid
The double C bond C=C alkene

C=C is from 1620 to 1680
but we dont really know that but notice the slope on the right side of the carbonyl is more gradual than on the left side. This looks like a serious clue we saw this earlier. Look @ a carbonyl peak for comparison. If you look @ the reference (Quickly and Correctly) you see the slope on the right should be even sharper. So this IS your clue.

What you have is a combination of a carbonyl and a C=C alkene combined. This is very interesting. The slope is an important clue for your instrument.

So something else important has been learned here. We do have a low resolution instrument & this is a part of the problem, but what has happened here is a combination of a carbonyl group and an alkene alkene. This is crucial.

With this knowledge, now we know that we have CH_2, CH_3, $C=O$, and $C=C$ and CH_2 has $n \geq 4$



$$\mathrm{H-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{C}=\underset{H}{C}-\underset{H}{C}=O}$$

but we are still not done

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Base frequencies p30
Strategy p30
Correlation Chart p29
Full Corr Chart p691
] Pavia

What are the base frequencies of C=O & C=C?

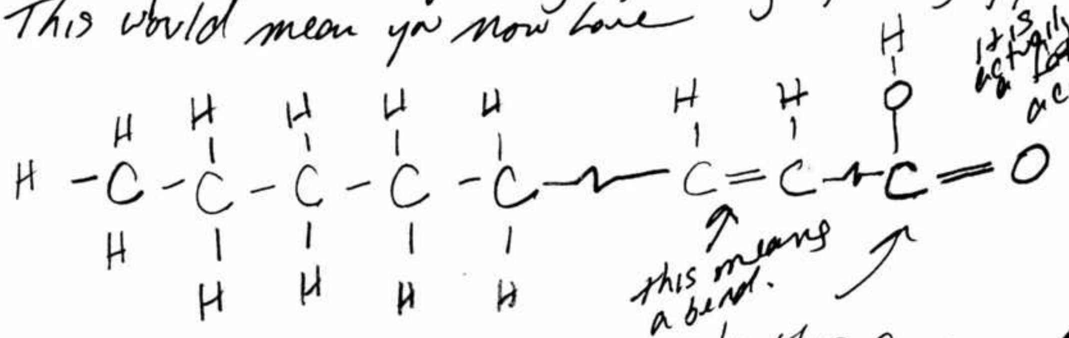
C=O 1715
C=C 1650

Our equipment just did not directly pick up the C=C. I believe the new instrument should.

Now lets look @ 1150-1160 peak again. This may have been a clue that we have a C-O bond eventhough we do not see an alcohol.

Now, IRSpec picks up on this situation right away. It identifies C-O in the middle of the band & even states an alcohol, but it does not state OH as an alcohol, it states C-O.

It says "C-O tertiary"
apparently it means three carbon neighbors
yes it does primary=1, secondary=2, tertiary 3, quaternary
This would mean you now have



It is technically ~~fatty~~ acid.

this means a bend.

This grouping is most likely to be split off on both sides.

In this case we have to wonder if tertiary meant 3 bonds to Carbon vs necessarily 3 Carbons

The net effect here, w/ a lot of adjustments + careful nuances, is that you were able to determine the essence of ~~structure~~ of the omega 3 fatty acid. But the alcohol group is somewhat baffling. What is the difference between a "C-O alcohol" and a "OH alcohol" ??
IR Spec is referring to C-O as an "alcohol" and my IR plot clearly does not show an alcohol and yet in a fatty acid you have a carboxylic acid but I see no evidence of ~~that~~ whatsoever in the IR plot of the fatty acid. Why?

It is saying that there is more than one way to get to an acid w/ IR. 10 pages of work to get here. Definitely no alcohol or carboxylic acid on my plot.

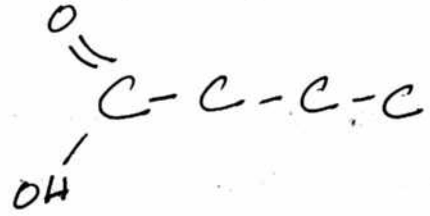
You still have to peak @ 1025 to take care of. Guess what. It is for a C-O alcohol again. This time primary. Which matches the truth. So this whole case is very interesting.

Ok, Lets Go Back to CBB Lipids w/ this knowledg
Apr 12 2015

Overall, it looks to be a simple structure.
With the line @ 3000
we obviously have C-H sp_3 bonds.
This gives us

C-C-CCC

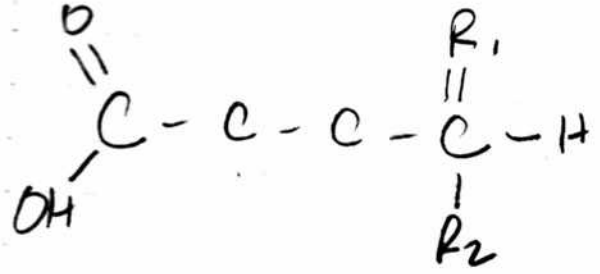
now we have the peak@ 2900 & ~2830
But you are missing the big picture
before you do this. you clearly have
the Carbonyl & the Carboxylic acid.
So now we have



the 2900 is an alkane, Fair enough, ~~also weak~~
Interestingly enough
IR spec has also picked up "methine"
here, which is actually quite specific and it fits
It is =CH-

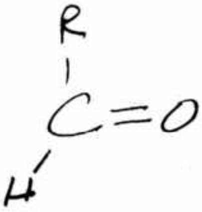
or

This Leads to

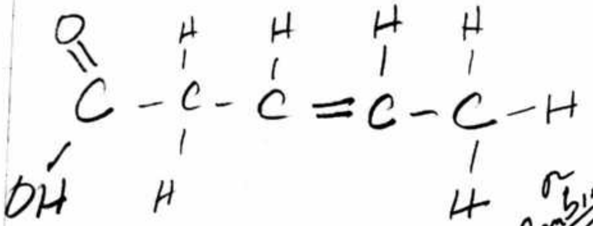


What we know is that we have a double C bond to something, but it could easily just be another carbon.

Now try to bring in 2830?
Aldehyde
Alkane - methylene (CH_2)
What is an aldehyde?

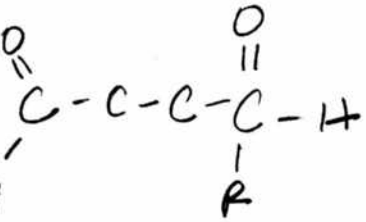


So we either have the structure to the right. A very good fit, or we just have CH_2
So we could have



or

or combined.



Now we see that something started to happen @ ~ 2650.
What is this?

Or you could have both!

For 2650
We get Carboxylic acid, amine or aldehyde.
It is interesting that we have a possibility of aldehydes twice now.

Remember:
We also know that it is likely highly conjugated and likely has iron attached.

Our next one is @ 1410.
Notice its unusual shape. May be
Combined factors or weak and broad.

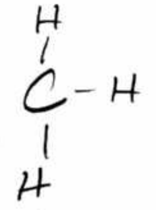
We get alkane (methyl) which
notice is CH_3

* This is not included yet.
~~We need 1270 next.~~
But we also get a nitro possibility.
N-O aliphatic
& N-O aromatic.
Stick w/ methyl for now.

Now we go to 1270.
We get carboxylic acid which is on. (1250-1300)
or Alkane @ 1260
This looks like a very good match to both.
This does not change anything.

Something happened @ 940.
We get an alkene. Looks good.
$C=CH_2$
a strong alkene.

So the parts are :



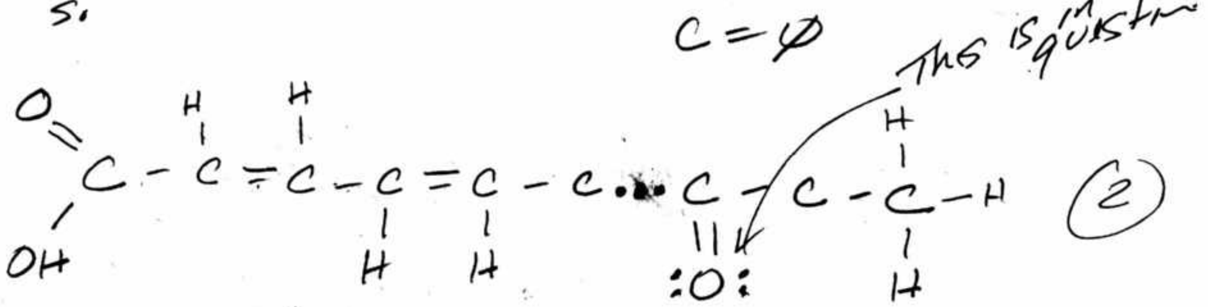
C=C

C=R

or

C=∅

So



THIS IS in question

②

what if this was C−C=O=C?

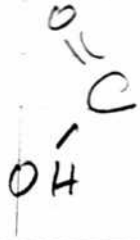
This is our proposed ~~structure~~ for the CDB lipids as of today Mar 12 2015.
It should represent an improvement.

It does, however, seem to make perfect sense. Next you need to learn about the reactivity of oxygen, free radicals, etc.
iron attachment, etc

Observed reactivity w/ halogen & iron are a factor in future development, along w/ improved instrumentation!

Lone pairs do not participate in chemical bonding - is that true? I doubt it.

So what if you have



"When fats or oils are exposed to air, they react w/ oxygen to form short chain carboxylic acids" The oxidation process is called rancidification.

Iodine reacts w/ the carbon carbon double bonds.

Remember also that you already have a $C=O$ bond in the carboxylic acid so this may be sufficient to account for its existence. You may not need to add any additional functional group.

Unsaturated fats and oils also react with hydrogen.

Like iodine atoms, hydrogen atoms "add" across the carbon carbon double bonds.

Saponification is also an important process

Salts of the fatty acids are produced.

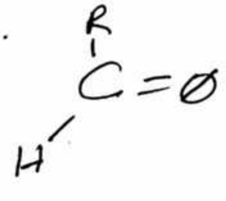
Oil + Water + Lye + heat should make soap.
& Cool it down, the soap floats

I see no reason to have a $C=O$ bond in the middle of the chain right now
Try to prove aldehydes.

What you did not do is work out the remainder of the list of Piavi Item #2 covering aldehydes, etc

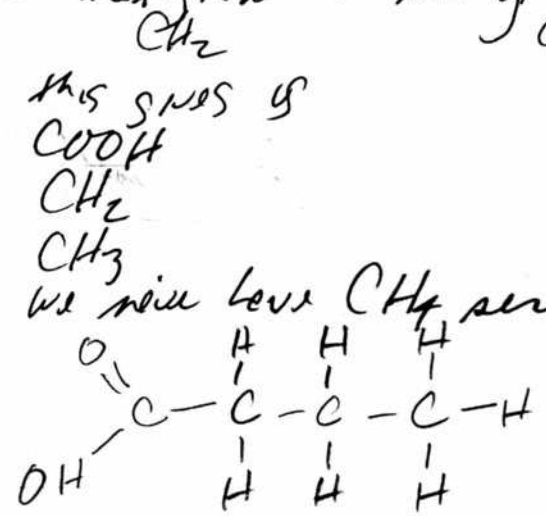
Lets review where the aldehyde & Extraneous came from.
2630

but before we go there, 2830 was our first hint of an aldehyde. Other than that, it was just an alkane of CH_2 which make perfect sense.
So then is a case where correlation on aldehyde would be important to investigate.
1st, what is an aldehyde?



You can not really justify going outside an alkane until all four on the alkane have been accounted for.
Koji tells us that we are entitled to CH_4 & H_2
Well, we don't really even use CH_4 and we don't really even have CH_3. Look @ IR Spec.
2900 methylene or methyl seem to be options. That is perfect
CH_2 CH_3
2830 methylene or methyl again
CH_2 CH_3

so this gives us
$COOH$
CH_2
CH_3
We will leave CH_4 since we do not need it.



Group
Frequency
Section

The mere dip @ 2650 reinforce COOH.

All stretch OK.

Now move to 1410. → This is where benzene ring is mildly possible

We get methyl or methylene again. So we confirm the structure further.

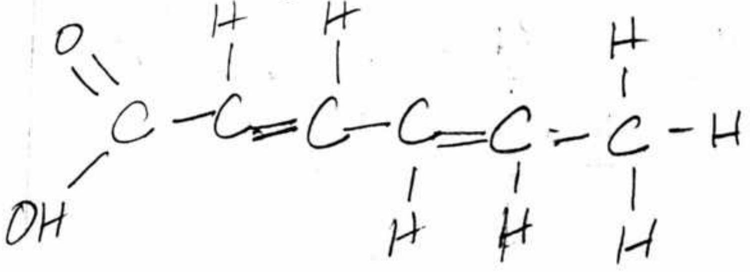
Now we go to 1270
We got Carboxylic acid again
& possibly methyl again.

We remain confirmed.

930 is almost our last move.
A definitive alkene comes in here.
This change to..

Benzene ring is possible but not more weaker than alkene

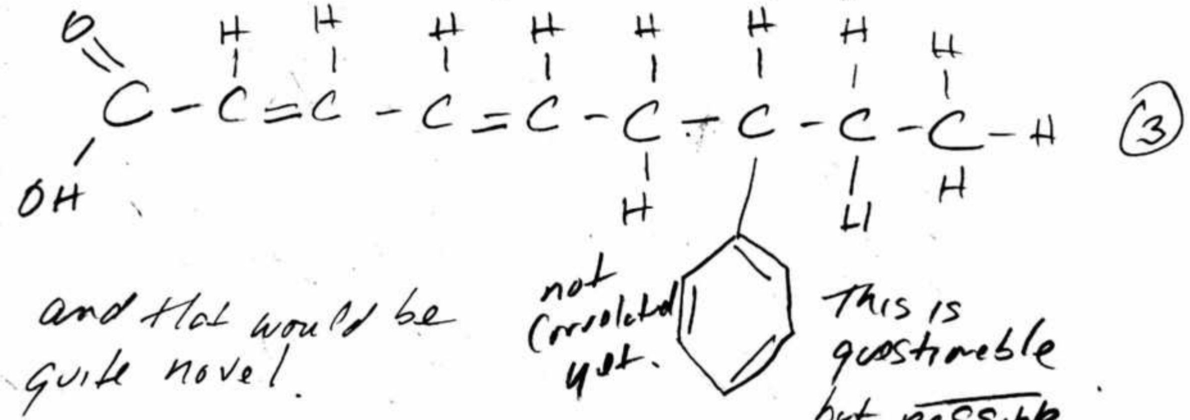
①



And the vis spectrum tells us that it is highly conjugated & this relates to the wavelength

Altogether you have 3 variation showing up and something else might happen @ ~110

We get an alkene again however the real Choice is a monosubstituted aromatic ring. This pose an interesting & unusual prospect of



③

and that would be quite novel.

not correlated yet.

This is questionable but possible

Now, do we not think there should be correlations w/ the aromatic? I would think so.
This is a Case for IR Pal
This might explain why Iodine hooks up so readily.

You need a little intreement to make ~~this determination~~.

This would be a "Cyclic Fatty acid"

Ok, we have made some real progress here w/ the interpretation of the lipids and we are learning a lott and also some of the nuances of our old very old instrument.

The IR spec progress is a very decent start.

Our Resources

April 13 2015

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Indeed we have very good sources to work with:

1. IR Spec (very useful first pass)
2. Pavia overview
   Pavia general foundation
   Pavia individual groups
3. Koji for some real detail
4. IR Pal for correlative work
5. Koji for some correlative work
6. ChemToolbox as an alternate table (not required)
7. Chem toolbox for many FGroup Illustrations
8. QUICK & CORRECT paper set!!! a Cincher sometimes!
9. Base value table
10. Workbook: Geometry, Formal Charge (headed toward Lewis Structures, Resonance, Acids & Bases)
11. Nuances of combined peaks & derivatives
12. Maybe a new math model as you wrap your head around these.

Follow up w/ these

Using these tools collectively in a smart sense is advancing your work considerably in IR Spectroscopy - keep it up.

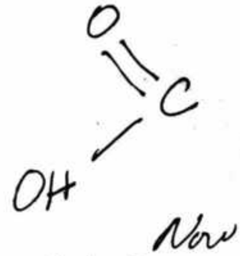
Now let's go back to urine:

[redacted] Urine: What do we see?
We appear to have a Carbonyl but notice that it is off center, shifted to the right. We also have sub peaks within it.

We also may have a very complex peak from 3600 to 2400. It looks like 3 flatteners combined.
1. Sharp dropoff @ 3600
2. Sub peaks across 3500 - 3200

So lets start w/ the sharp drop @ 3600.
Now, 3200 - 3600 is an alcohol so this looks like a major candidate.
But what we really have here is a Carboxylic acid.
Quick & Correctly (better name = quick & easy!..)
There definitely appears to be a Carboxylic acid from quick & easy but there is more going on with the sharp drop @ 3500.

It appears that we have an OH separate to but also combined w/ COOH
It seems to be too powerful.



and OH separately.

Now we can look @ the sub peaks

3450 Amine (3300 - 3500, medium)
3330 Amine (3300 - 3500, medium) Could be Alkyne C≡C-H
3190 Amine, Alcohol, Carboxylic Acid.

[redacted]

So now we anticipate

OH
separately

N-H
primary ?
secondary ?
tertiary ?

Lets see if we can zero in on the amines

3450 ✓ works perfectly for Chem Toolbox
3330
3190

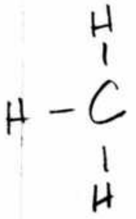
Lets work on this in detail from various sources

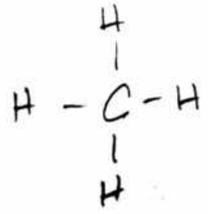
Chemistry Toolbox
~~3540~~ 3460 - 3280 - amine
N-H stretch · 2 bands
What does the "1° amine" refer to?

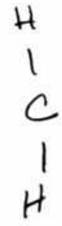
ChemTool Box has an amide from 3180 to 3200 but it is 2 bands within which we do not have
So Caution Here
There are still some questions here on 3190

Koji 3190 candidates are also lacking here
Primarily the OH and amines are the main contenders, and the amine & alcohol this is OK. Amine is probably the stronger of the two.

So what do we know so far?
We appear to have



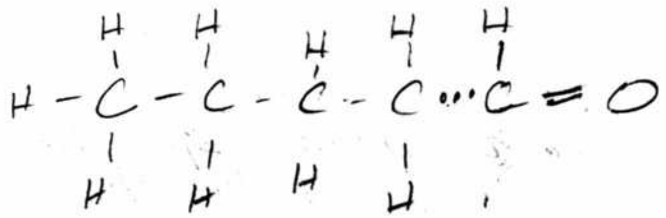




and C=O

and $n > 4$

This suggests something to the effect of

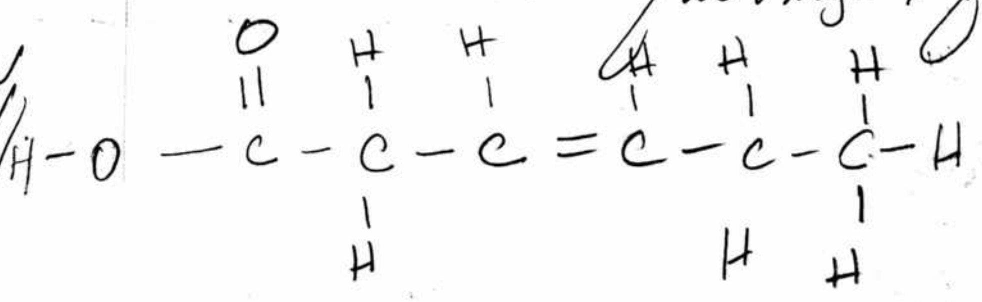


This means the oil is unsaturated.
Now we would work in the fingerprint region.
~1150
~1020

IR Pal 1150 is full of options but
The ester looks like a possibility
RCOOR

The actual structure of an omega 3 fatty acid is

ACTUAL



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Koji seems the most detailed

3450 Either $R-NH_2$ or $Ar-NH_2$

3330 $R-NH-R$

3190 Difficult to assign.

Looks like best candidate is $C=NH$ (3400-3300) w/ $C=N$ correlation @ 1690-1640. Which we do have.

So we seem to have several contenders here.

$R-NH_2$ and $R-NH-R$ and $C=NH$ and $C=N$

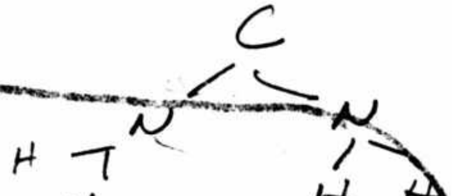
So on the table now is:

OH separate

$N-H$
and/or $R-NH_2$
and/or $Ar-NH_2$
and/or $R-NH-R$.

$C=NH$ $C=N$

We know we have



but we certainly seem to have more going on than this.

Now progress to 1640.

We are getting $C=C$ or $C-C$ or $C=O$ and $N-H$ or Acyclic Alkene or Benzene Ring

Lots happening here

Now we have 2 small subpeaks @ 1660 & 1615

1660 We could have a benzene ring (1660-2000) weak. or an alkene

1615 Amine $N-H$

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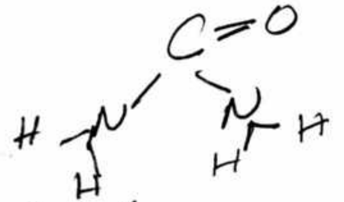
Knowing



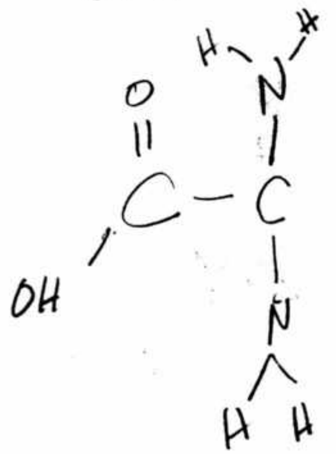
Many many Candidate now Coming in.

C-C   C=C   OH
separate

NH
R - NH_2
Ar - NH_2
R - NH - R

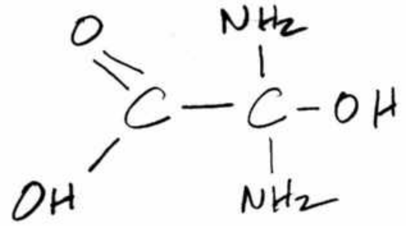
C=O

Aromatic



Our simplest Combination is

This is possible it seems:



w/ possibilities of additional
C=C
~~OH additional~~
Aromatic

This all seems very realistic.

Look @ this statement

" However, amino acid degradation can produce uric acid or ammonia instead "

under amino acid - wikipedia

This statement is critical

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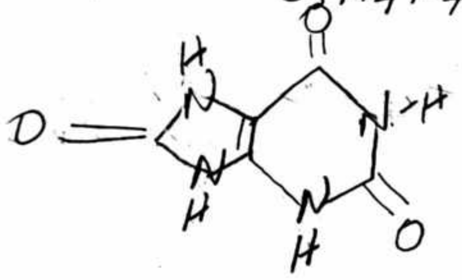
Uric Acid $C_5H_4N_4O_3$

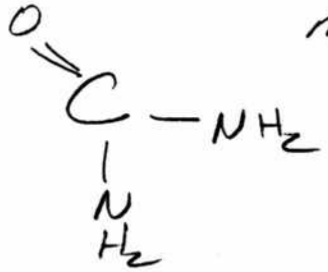


Is it really a benzene ring? As a structure it would seem so.

A "heterocyclic compound"

Why no alcohol functional group? An interesting question – it is a peculiar situation.

So I would have both urea <u>and</u> uric acid.
not both.



Now lets move on to the next set.
1445 alkane (true) or benzene ring (true)
1140 Alkyl Halide (not known) or amine (true)

You therefore have a very good ~~determinat~~– that of ~~lead to an~~ characterization of both urea and uric acid in the urine sample.

And remember the statement in black on the left & then ASK how does the degradation occur:

Apr 13 2015
Now Lets go to blood again.

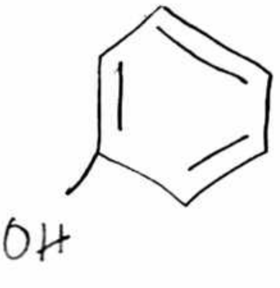
The most striking feature are the huge bands from 3600-2400 and 1800-1000. These are massive hard & suggest combination.

Now there is no Carbonyl!.
But is there an OH.
He immediately check for alcohols & phenols.

Left: seems like it might be a combination of alcohols, phenols, hydrocarbons and/or aromatics

Now from Pavia, ~~alcohols run from~~ acids ~~from~~ run from 3400 - 2400 (which is what we have) and overlap CH. This fits in very well since it looks like we have a combined peak. But we do not have a carbonyl group. This indicates an acid but not a carboxylic acid. What we know is that phenols are much more acidic than alcohols but not nearly as acid as carboxylic acids. So immediately phenols, aromatics and hydrocarbons come to the forefront of the list.

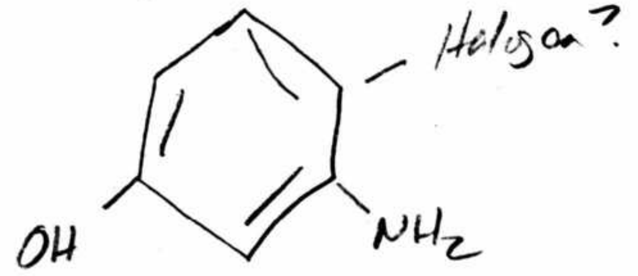
OH



C-H

Now lets look @ the sub peaks
3250 OH, Amine NH, alkyne, Amine
2920 amine, alkane, maybe alkene

This suggests



Now we go to 1500. This is a very strong peak w/ what looks like a fair amt of activity around it.

1500 Benzene Ring @ the top of the list.
Also N-O aromatic
alkane
Nitro N-O aliphatic

This gives very strong evidence to support the phenol group w/ NH2 attached

We have some activity @ 1275
C-O (This would match OH attached)
and a Carboxylic Acid also but
we have no Carbonyl ??? This is a weak peak.

600 C-Br
C-Cl
alkene
Benzene Ring monosubstituted

550 C-Br
C-Cl
C-I alkene

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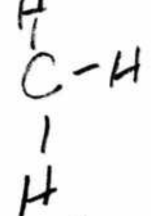
Now lets go back to [redacted] blood & look for difference.

the low spot on the main peek is 1515 VS 1500 on mine.
Benzene shows up for both so no change there.

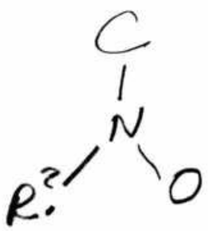
Next [redacted] has a 1400.
We did not.

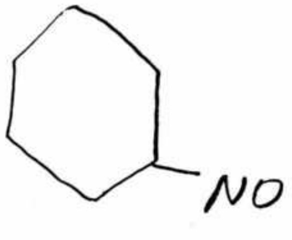
1380 1400 weak Alkane C-H methyl
1380 weak Nitro N-O aliphatic
1350 Nitro N-O aromatic

So we have a new twist introduced here



methyl





Now we move on to 1300 w/ [redacted]
(I did not have this)

Possible 1300 1250-1300 Carboxylic Acid C-O
1100-1300 Ester C=O

Seems less likely water band
These are interesting also but they
1260 alkane - methyl

possible again
do open up interesting prospects also.

Queston here.

This last result suggests that the Carboxylic Acid now should not be discounted @ this time. IR spec lists the Carboxylic acid as a C-O not a C=O !!! What does this mean? This could be important. Can you have a Carboxylic acid under a C-O and not have a Carbonyl group C=O ????

So a new question here

Can C-O be associated or ~~interpreted~~ as a Carboxylic acid.

Blood pH is so narrow ~~that~~ it seems like a Carboxylic acid in the blood would be truly problematic.

The methyl alkane may end up being the lowest common denominator.

I think the message here is that we have some activity in this region (1600-1100) that will need to be sorted out.

And you have a question about what Carboxylic acid actually infers. C-O and/or C=O

[redacted] may also have some activity @ 925 not duplicated anywhere else yet.

It could be an alkene which is nothing new.

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Now we repeat the CDB-Blood Mix

The difference from a reference that we see here are

Possible @ 2000: interesting Properties here
Alkyne $C \equiv C$ (2100-2260)
Isocyanide (that's new) R-N-C (2110-2165)
these are interesting:

$C \equiv C$
Alkyne

R-N-C
Isocyanide
(What does this mean?)

Now we also have new & strong peaks @
more likely 1640 Alkene (1620-1680) C=C med to strong
less likely N-H Amine (1560-1640) strong

weaker 1525 Benzene Ring (1450-1600) weak
more likely Nitro & N-O Aromatic (1520)
possible Nitro N-O Aliphatic (1540) Strong
no idea Amino Acid (C=O Zwitterions)

look @ correlations here w/ IPA

[redacted]

Next we have
1400 1400 This activity repeats from [redacted]
1300 1300 This activity repeats from
new → 1120
C-O Ether aliphatic (1120)
C-N Amine (1020-1230)
C-F Alkyl Halide (1100-1200)
Ester C=O
C-O Alcohol

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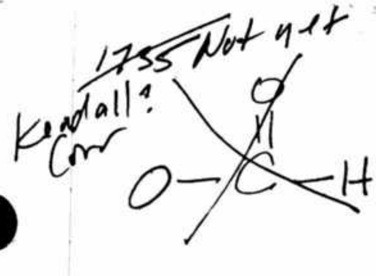
Kendall Corr Chart p211
Kendall Outline p182

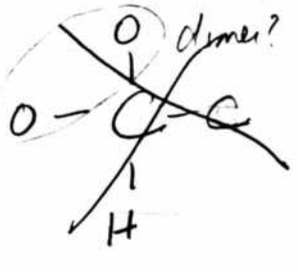
Apr 15 2015 Going Back again Omega 3
This time with Kendall (Back form & Corr Table)
The heart for us is Ch5 p166 & the Outline is on p 182
5000 - 1333.

Now w/ the 3000 line, the primary as well as the sub peaks indicate the C atom is saturated. His definition of saturation means tetrahedral geometry Maybe it could be any type of bond
Now our two major peaks are @ ~3000 and ~1700
Our numbers on the strongest peaks are
2900 Interesting. ~~Kendall shows CO_2H dimer (what is a dimer)~~ → NO!
Which is different than anyone so far.



This is a perfect match.
But ChemToolBox gives (2850-2980)
Alkane, straight & simple
C-H stretch, 2-3 bands
which matches perfectly.

Sub peaks are @ 2980, & 2820
The width of the major peak is 2800-3000. This width & slopes are also important
What if the dimer did not have a ~~d~~ double bond, then it would be fine.



Not true, Kendall has the BIG PICTURE @ the top of the Corr Chart. You missed it.
Clearly states C-H stretch.

· IR spec also show alkanes as strong.

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Quick, offline sources are becoming
Book hardcover

Blue fire Kendall phone → ChemTool Box (Online once)
IR Spec → Pavia (Blue reader)

We can flop between phone.
So am arrangement is:

① Phone: IR Spec
ChemToolBox if you can get it once
Flip between these w/ task Manager

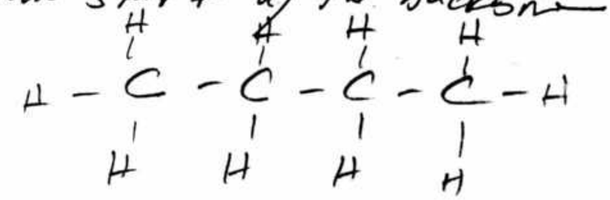
② Bluefire can have Pavia up

③ Kendall is hard cover

④ Quick & Easy (paper set when you need it)
⑤ Koji as defining support
⑥ Base values (for reference) as needed.
7. IR Pal is available (if PC is available

So back to Omega 3.
Major peak @ 2900
Sub peaks @ 2980, 2820
Base value for CH is 3000, so that seems pretty Straight forward. Left of 3000 is unsaturated, right (<) 3000 is saturated. We are right, so we have saturation (saturation here does not mean all hydrogen, it means all bonds occupied.)

So we can start w/ the backbone



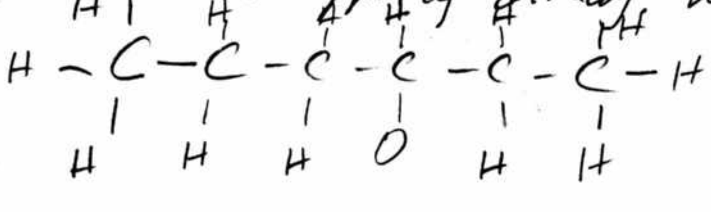
Quick + Easy also confirms this back

~~Now we go after to second main peak~~ This is @ ~~1130~~

actually we see that w/ Kendall we should follow the alkane through + pick up the additional backbone structure.

He has 1455 (we have 1440) as CH_3 and CH_2
He has 1375 (we have 1365) as $C - CH_3$
We have it.

Now, with Pavia, his flow chart led us to a C-O bond with an ether
So, lots is happening already. We may have



the 725 band (we have 690) may also indicate 4+ methylene

and this was fairly quick. By Kendall, we suspect presence of an aliphatic compound, possibly w/ an Oxygen attached.

The next broad feature we notice is that the slope of 1715 on the right side decreases.

We see from QUICK a look that this does not happen w/ a Carbonyl. In fact a Carbonyl is usually around 1700. So this indicates a combined influence of some kind.

What happens around 1680 ?

IR Spec ~~Toolbox~~ gives us

1650 C=O amide

1620-1600 C=C Alkene medium to strong

We are also getting mention of acyclic alkenes.

Toolbox gives us

1630-1600 alkene C=C a good match.

So the evidence for an alkene

The 1300-1000 range, and we have this as well as 1160 peak gives Pavio C-O bond (ether). What is an ether?

An ether is

Toolbox@

1160 w/ Range 1110 - 1290 (matches)

also gives us an ether as C-O-C

Peaks:
2900
2980
2820
1715
1440
1370
1160

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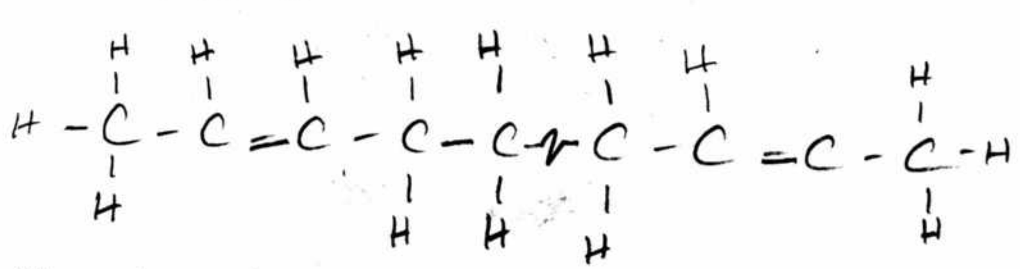
The 1160 is getty pretty strong.
So

C-H
$C-H_2$
$C-H_3$
C-O-C
C=C

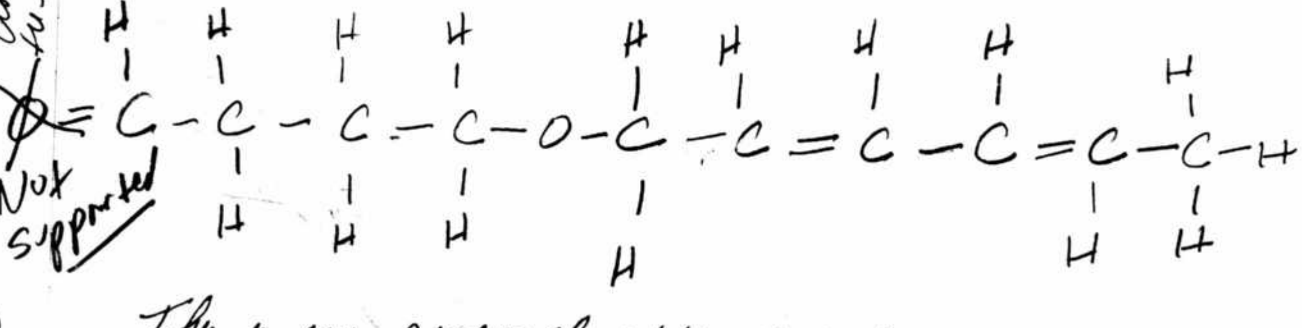
$n \geq 4$ is likely.
No alcohol or carbonic acid
which is interesting on a commercial
fatty acid.

Also the base value for C=O is 1715 you can't get any better than that @ 1725 so now
C-H, $C-H_2$, $C-H_3$, C-O-C, C=C, ~~C=O~~

We have an additional piece of information @ ~~1125~~ 1025.
Toolbox Corner and strong at a C=O.
So this is consistent



Now, to work in the C-O bonds we have something like



Not supported

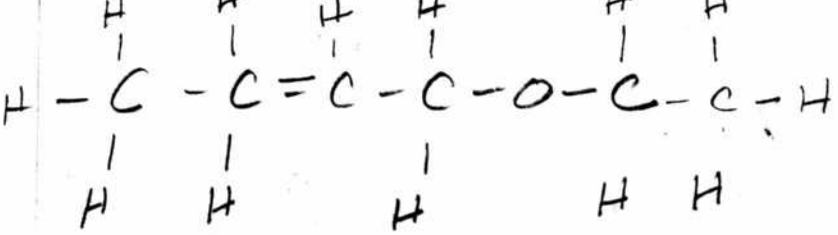
Can oxygen make a double bond by itself at the end of an aliphatic chain.

This is our proposal w/ the caveat on oxygen! You found a mistake
1025 not 1125!

IR Spec ~~Toolbox~~ Notice: alkenes go up to 990-1000.
I vote for this..

Toolbox also has it.
Simplest explanation is bending motion of an alkene

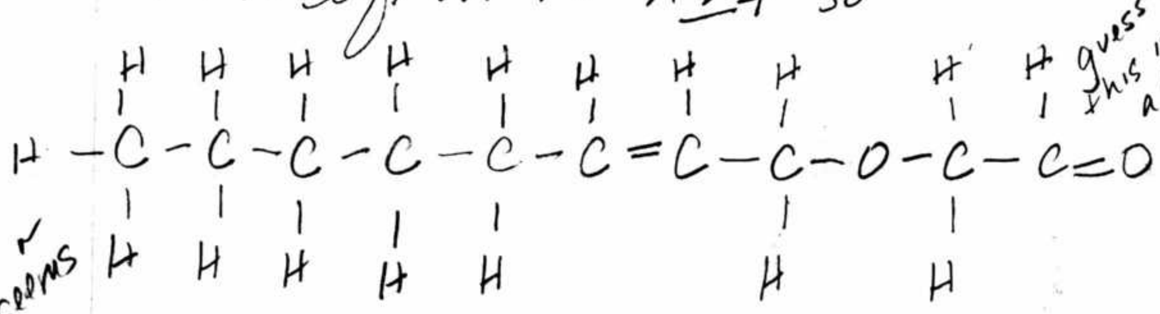
So now we have



No alcohol or acid present

The proposed minimal structure of the Carol Version Super Omega 3.
Now we expect a higher level of conjugation

But we left out the $n \geq 4$ so



guess what, this is an aldehyde!

no alcohol or acid seems to be present

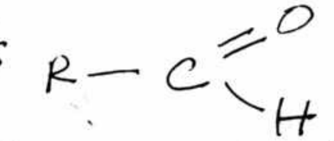
Then a now our proposed ~~structure~~ for our Super Omega 3 fish oil
Conjugation could be much higher.

We have a functional group chart
on p17-19 in Barrows
Organic Chemistry!

Continuing, our peak @ 1725 Needs further examination.

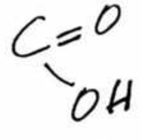
First: a definition: a carbonyl group is called a C=O bond
Now we surmise that we have a combined peak @ 1725

Now Toolbox clearly gives us a C=O in this range (up to 1725)
IR spec also front of center gives us a C=O clear as can be.
We also, from IR spec have a strong candidate of aldehyde (1725-1730) range.
so lets see what an aldehyde is:

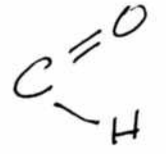
aldehyde is  Can be

This is actually very interesting because it is so close to an acid. The range is also a strong candidate

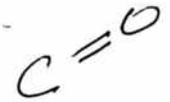
Notice



acid



aldehyde

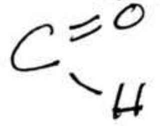


ketone

Notice the sequence of dropping
Acid, COOH, drop the O get an aldehyde, drop the H get a ketone

You now know a very useful relationship
between acids, aldehydes & ketones.
This is great.
And they <u>all</u> have a carbonyl.
ketone is the simplest C=O
aldehyde adds an H
acids are a COOH (added another oxygen)
Very cool.

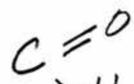
So there is a case where a correlation
chart is very valuable.
The question now is, what correlates
w/ an aldehyde?



I think
IR Pal is our only
hope for Correlation <u>work</u>.

Correlations w/ aldehydes are:

2720
2820 <u>Yes</u> we have this!

Now we know
$C-H$
$C-H_2$
$C-H_3$.
$C=C$
aldehyde 

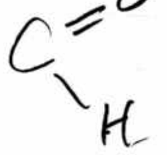
$C-O-C$ needs to be proven.

So what happens here is that IR spec Comes up w/our best candidate & IR Pal Checks for Correlations.

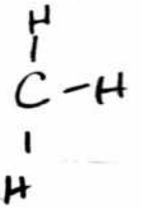
So now from scratch, we'll have 2900 & 1725

IR spec Comes up with carbonyl & aldehyde right away. for 1725.
IRspec IRspec

Now for 2900, IR spec gives COOH which we know it is not. It also suggests amine which also is not good.
Then it immediately jumps to alkane very strongly w/ methylene @ 2925 (very close)
methyl @ 2870 (very close)
and methylene again @ 2850 (also good).
So now we know we'll have



IR Pal Confirms @2820



IRspec

IRspec

IR Pal all across the board

IR Pal gives
1460
1365
& 722
Correlation

The next major feature we noticed is that the slope < 1725 has been modified. This means something is affecting it. What is affecting it is in the range of 1600 - 1700.

1650 area IR Spec

Either an amide or an alkene
C=O C=C
so a double bond is affecting it. Which one?

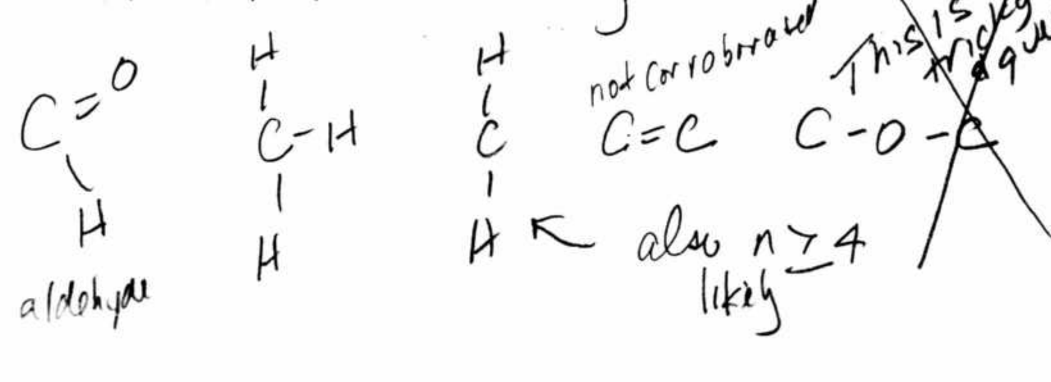
So now look for correlation on IR Pal

on ethers
A big difference!
Toolbox

Amide correlation is not working well. Nothing to corroborate it but so far an alkene is the stronger candidate

1110-1285 So now we keep working it.
1070-1150 from IR Pal 1150. Now this is where the tools get interesting. Here the first target peak, rather than a range is C-O aliphatic, an ether.

What is an ether? An ether is C-O-C
So this is where we bring this in.



aldehyde

not corroborated

also n ≥ 4 likely

This is tricky & questionable

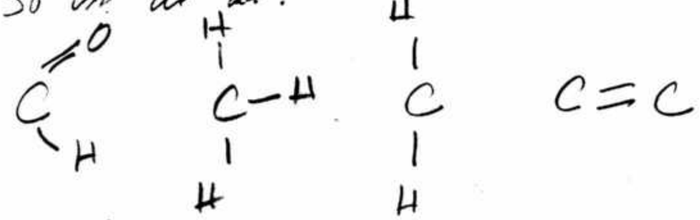
not substantiated

Next we move on to 1025

Before we do this, we need to square away on the range of ethers. Go to Koji's

This 1150 is all over the map.
  Koji has CH_3 I don't buy this.
  IR Spec does not
  IR Pal does not.
IR Pal has a slough of inorganics.
  Koji, ketones, esters, ethers.

I think this is hard to assign.
  So it could be ethers, ketone, esters
Since a ketone is $C=O$ this could be our simplest case scenario. It is to be adopted @ this point.
So we are at:

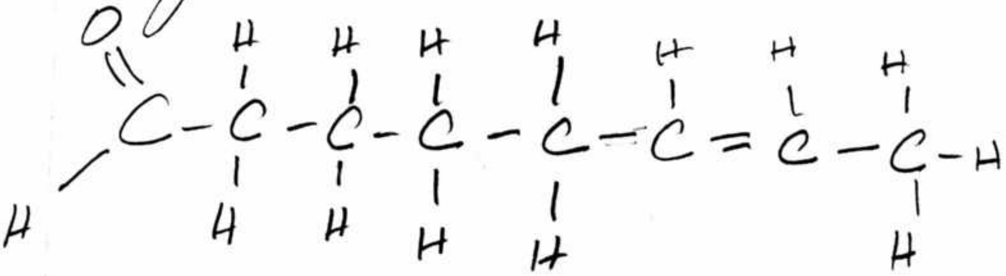


$n \geq 4$
likely.

Now we go to 1025.
  IR Spec, no alcohol, amine evidence
Alkene comes in strong @
But also, what is a primary alcohol?
  There is no evidence of an alcohol.

Omega 3 Result

Therefore, we are now led to:



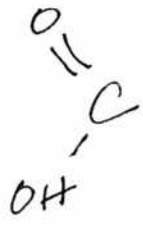
This is the minimum configuration that satisfies all conditions and that explains the lack of an alcohol & the similarity to an acid.

It seems as though the omega 3 product may have been altered to some degree.

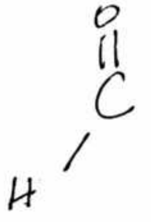
This seems to be our best work yet and also on very solid ground with no real speculation ~~taking~~ place.

Your work on the aldehyde was good here. A better understanding of carbonyls & their progression from

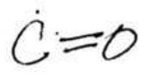
COOH COH CO



Carboxylic Acid



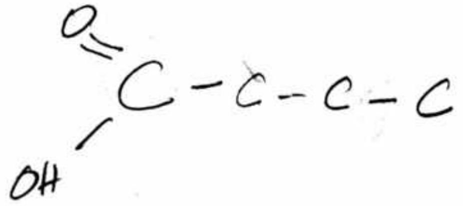
aldehyde



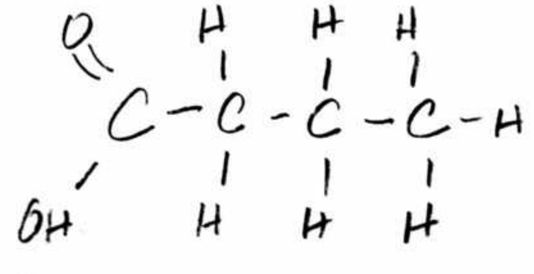
Ketone

Now we can legitimately move on to COB Lipids again. We have some similarity but there are some important differences

We have the major alkane peak @ 2900
We have a clear Carbonyl @ 1700
We also have a clear Carboxylic acid so



Now look more closely @ 2900 & ~2830. Sub peaks
IR Spec
2900
Carboxylic acid. Strong & agree
We also have methylene @ 2925
methyl @ 2870
And these all make sense. So we expect

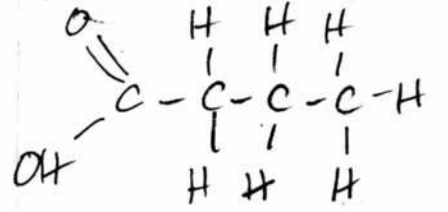


Now we have something medium @ 1410 that looks like it might be combining two peaks.
So the simplest here is alkane.
But we have an interesting case from IR Pal.
A Sulfate ester S=O
and the range is 1350 – 1450

Toolbox gives both
$\bar{Y}$ = 1380 an aliphatic aldehyde (1320 - 1440) H-C=O
$\bar{X}$ = 1395 and sulfate S=O stretch (1450 - 1340)

so these are both very close
Now IR spec does not have either one
of these but they do have the alkanes (bend)
which we have already identified in
the omega 3.
So something is different here. and
is being attached to the alkane peak
to broaden it out.
It should be something right @ 1400.

The sulfate is a little closer.
So we now have



and

H - C = O
or
S = O?
S - H?

Interesting

Now notice we had a little activity @ 2640
Looks pretty weak. (2540 - 2600)
Toolbox Possibly a Thiol, which is a S-H stretch

but IR spec gives an aldehyde @ 2720 not so good.
IR spec gives only organics.

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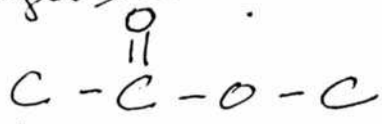
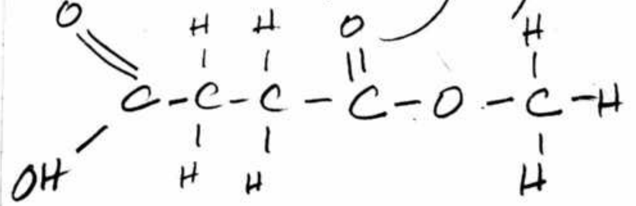
Now move on to 1210.
Looks like a Carboxylic acid.
Straight.
But it very much could be an ester   IR Spec
It is a strong peak.   two bands
We may have a merger here.

An ester is


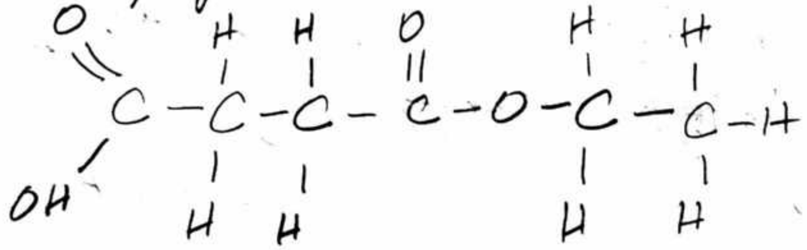
$\mathrm{C-\overset{\overset{O}{\|}}{C}-O-C}$

This makes perfect sense
This would really open things up.



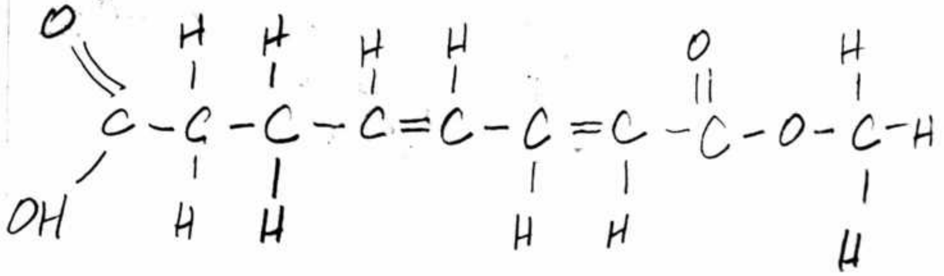
and $H-C=O$
or
$S=O$
$S-H$

So propositions:



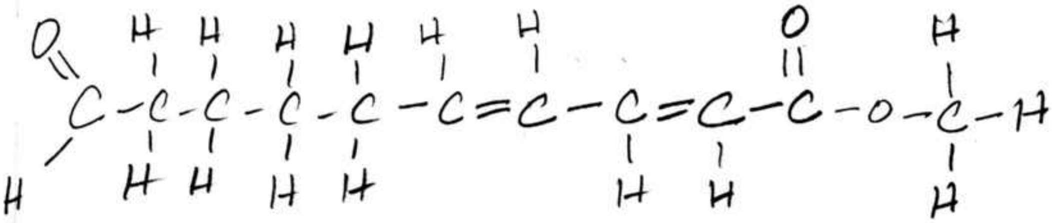
$H-C=O$
$S=O$
$S-H$

Now 930 is the alkene $C=C$



Oxygenated, unsaturated, fatty acid

And now something has also happened @ ~710 and this is the ~74 for the alkanes. CH2 So now the chain gets extended ..



And this, Dr Watson, is the currently proposed introduction to the molecular ~~structure~~ of the CDB Lipids

" long chain of poly- Unsaturated oxygenated fatty acid "
highly conjugated

Potential Problems

Oxygenated - Oxygen steals electrons
Reactive w/ Halogens
~~May~~ Subject to oxidation
Endotoxins are possible if not likely
Lipid peroxidation in the presence of free radicals

an alternative interpretation of oxidation

When oxidation is taking place, an element is combining with the oxygen

The Tools, System & General Strategy.

Our tools & system are now:

1. IR Spec - initial estimates
2. Chem Toolbox - 1st Corroborations (initial net connection)
3. IR Pal - Further correlations, additional prospects (PC)
4. Quick & Easy representative plots
5. Koji Corroboration
6. Pavia flowchart & elaboration
7. Kendall flow chart & elaboration
8. Base values are always of interest
9. Strive for lowest common denominator - avoid speculation
10. Consider derivative & combination effects on a continual basis.
11. Examine subpeaks within major peaks.

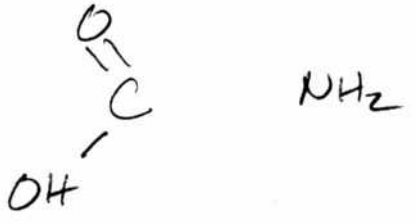
Now we can continue - urine
Testing this pen.

So far the major feature < 1337.

A combination of N & COOH it seem on the surface
w/ A carbonyl group
So main peak is ~3500 to ~3100

3300 - 2500 is Carboxylic so we certainly
seem to have that.

But something started @ 3600
So now we are looking @ 3600 - 3300
This appear to be an amine (3460 - 3280)
So now we see

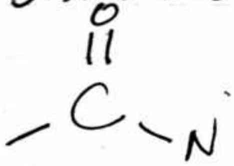


Now we have 3 subpeaks @ ~3450

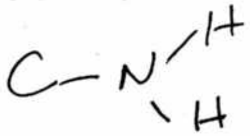
IRSpec Toolbox	3450	Amine (3300 - 3500)	medium
		Amide (3440 - 3420)	
IR Spec Toolbox	3350	Amine (3300 - 3500)	medium
		Amide (3360 - 3340)	
IR Spec Toolbox	3190	Amine again (3000 - 4000)	
		Amide (3180 - 3200)	

So what is an amine vs an amide?

Amide is



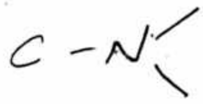
Amine is



Now there is a split of opinion here. I think that toolbox wins because they are so specific & match so well.

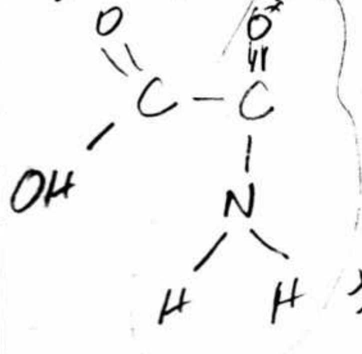
So this indicates

amide is more specific



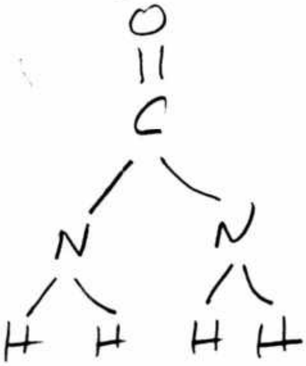
amine only requires C-N

Ok we have learned some important things from this round, Assuming you have a single compound can be very problematic. It mixes things into one when it is not justified, eg



I picked this up perfectly

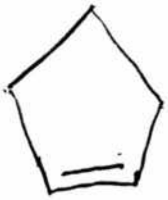
but we know that Urea is →

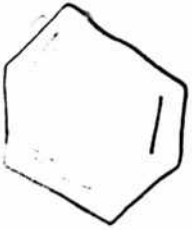


Now lets move to 1650.

We have a mgn peak @ about 1640
with a range of 1725-1500.
This should be associated w/ a carbonyl
COOH? COH? CO?
Car. acid aldehyde ketone

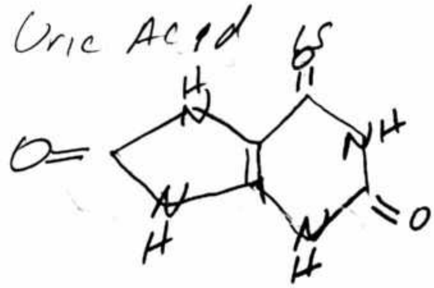
Toolbox: Gives best fit as
Carboxylic Acid (1740-1680)
Now it looks to me like we have a
Combination effect since the peak is
shifted. We also have 2 sub peaks.
The sub peaks are at
Strong Candidate
IR Spec 1640 Acyclic Alkene, alkene, Carbonyl
Benzene Ring
1610 Amine, Amino Acid, Alkene,
Benzene Ring
So I believe we have a ~~Carbox~~ carbonyl
group (Carboxylic acid) joined with
an acyclic alkene.
So what is an acyclic alkene?
They can be 5, 6, or 8 sides
they seem to have just one double bond





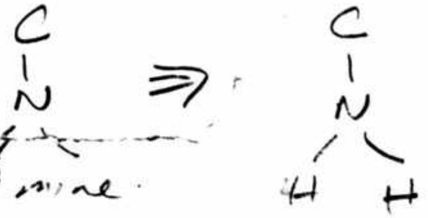
You have really nailed this
haven't you -

Uric Acid



We now have

amide

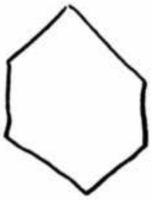


Amine
Primary

C=C
alkene

C-C tri/tetra substituted

Now we pick up a benzene ring @ 145? IR Spec
↑
Tool Box is not picking this up at all.



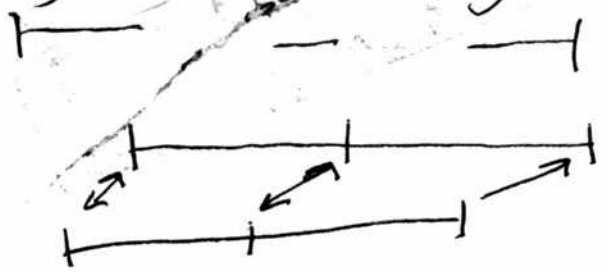
Could also be alkane, methylene (CH_2)?

Program - Spreadsheet Ideas
If we were to develop a spreadsheet
what would we do?

First we seem to hold over to 1k spec first.
What are you doing there?
It makes a difference if something is a major
peak or a minor peak.

If it is major you are looking @ whole range.
If it ~~is minor~~ you are looking @ a number
in a narrow range.
It affects what candidates you select.

Your selection of theoretical range value
pretty much tells what you are doing.



These differences give you first estimate as
to how you are doing
but 3% is a lot of error it appears
eg what is 720 vs 690? 4.1%
So yes 3 should be a trigger.

% error	Score (Decimal)
0.001	1.00
.5	.95
1	.90
2	.80
3	.70
4	.60
5	.50
10	.05

Linear solution is good.

Score (decimal) = $-.095\overset{*\%\text{error}}{4} + .9916$ ~~* % error~~

$r^2 = .\underline{\underline{999}}$ good <u>model</u>

OK, you have a range analyzer set up.
Now, how t approach probability.

1 Score = 60 %
2 Scores = 55 %   The 55 is probably better than the 60
how would you determine this? Joint probability?
Seems like it is close to $(P_1 \bullet P_2 \bullet P_3 \ldots)^{1/n}$??
No, not really.

Ok, you apparently have worked out the probabilities
of multiple occurrence.
Now you need to figure in fingerprint.

Fingerprint wt = 1
Group wt = 2

So if you have an 80% in Group
how does this compare to a 80% fingerprint?
It is better. How much better?
Twice? No $\sqrt{2}$ Maybe about right.
What about 100%? you can't get much better than 100%

$100 \cdot \sqrt{2} = 141.42$

Ok, we have a model to start working with
It considers
1. Range matching
2. Correlation ~~&~~ No Range matching
3. No. of correlations
4. Group a fingerprint location
5. Derivative influence & ~~interpretation~~
~~of combination influences~~.
6. Combination influence.

Apr 16 2015

Let's ~~start~~ simple w/ model & see how it does

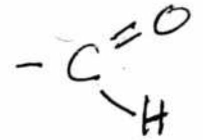
Urine Analyze w/ model Apr 16 2015

Major peak
Range is 2800-3000 Peak = 2900

Nothing shows in IRSpec
Toolbox:
Alkane shows up 2850-2900
Enter it in model

Now we have sub peaks
IRSpec 2900 2975 Alkene =C-H_2
2900 2925 Alkane CH_2
2830 2820 Aldehyde C-H

Aldehydes are actually



OK, you have these in your model & they look very decent.

IR Spec

Move to the carbonyl.
meas 1675-1780 Range Peak @ 1725
IRSpec Carbonyl 1670-1780

Aldehyde 1725-1730 saturated.

Work on right slope of carbonyl—

Now lets move to the projected Carbonyl

we have the range in place.
Now go for the peak.

1730 IR Spec has it @ 1735
This is a Carboxylic acid.
But we donot have the wide peak to support this.
An alternative is an ester C=O @ 1735
Ketones @ 1715-1720
Ester again @ 1715 but this might mean a double peak.
aldehyde @ 1705

We missed the primary target
IR Spec has aldehyde @ 1725-1730
Right on the mark

and we had it in the spreadsheet. So we are right on the mark.

Now lets look @ the altered slope
Something changed from 1690 to 1590.

Out of curiosity, notice slope also changed from 2800 to 2600 what might be happening here?
2720 is aldehyde again! IR Spec C-H
vs our 2730

We know that the 1.41 factor can be simplified from what we have.

Next is still in fingerprint region we have

1440   IRSpec 1470 alkane
no real competition
1365   1380 alkane

other competitor showing up is nitro @ 1380
but this should have resulted in a strong peak @ 1560 which we do not have
alkanes win here.

Now we are in fingerprint region.

1155
Ok, but we actually have a range here so take it first:
1200 – 1125   Center = 1160
Not a great match on ranges in IR spec.
Go to Toolbox
No immediate matches.
.Extend range from 1125 to 1265
IR Spec is (1100 - 1300)
One possibility here is an ester.
but it also has two bands

SPONCH

This band @ 1155 is more problematic.
Either a new organic (with weaker or lesser
or no corroboration) or an inorganic
consideration

IRSpec Candidates: Alkyl Halide
Ester C=O OK for range
but two bands (we don't have this)

An ester requires ~~colta~~ correlation @
1840 (none)
1730-1780 (maybe just fine here)
This could explain the shift on the carbonyl

Toolbox 1720-1765 C=O Excellent match here.

Therefore ester does have some important correlation

The next is @ 1035
The range here is 1000-1070
IR Spec has no good match.

Remains Open

We have no good match here.
from either IR spec or Toolbox
We may be dealing w/ an inorganic here?
Akyl Halide is showing up some twice now
C-F?
It did show up but required two bands @ 1155
This can not be entirely dismissed.

So our options are to
1. add the alkene @ 670-700
which is a good match
2. ignore the three peaks @ 1155, 1035
& 690 as producing an
alkyl halide w/ some ambiguity
in Cl, F, structure.

a

adding, propose & compute the
halogen probability.

At this ~~case~~ point, also knowing the sample
type, the conservative approach
is the former. Add the alkene.

This means that the only unresolved
peak will remain @ 1035.
This can be studied further @
your discretion

So we measure 690
w/ range ~~known~~ of 600-715. =C-H

IR Spec 670-700 strong

The Spreadsheet Program
Appears To Be A Complete Success
Results Duplicated Exactly.

Therefore our final probabilities are:

C-H Alkane 100%   CH~ ~~3000~~, 2900, 1440, 1365 methylene methyl
methylene CH_2

C=H Alkene 70%

C=O, C-H aldehyde 100%

C=O Carbonyl 100%

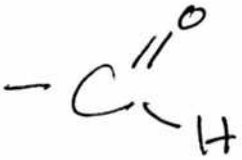
C=O, C-O Ester 69%

Now we need more specifics on each structure.

100% Alkane: We have CH_2, CH_3 & sp^3

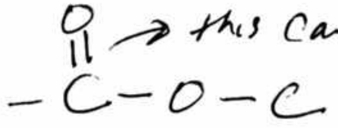
70% Alkene We have $=C-H_2$
$=C-H$ (subset of above) but notice C=C cause this to happen so it may be distinct

100% aldehyde



100% Carbonyl C=O is a subset of above aldehyde

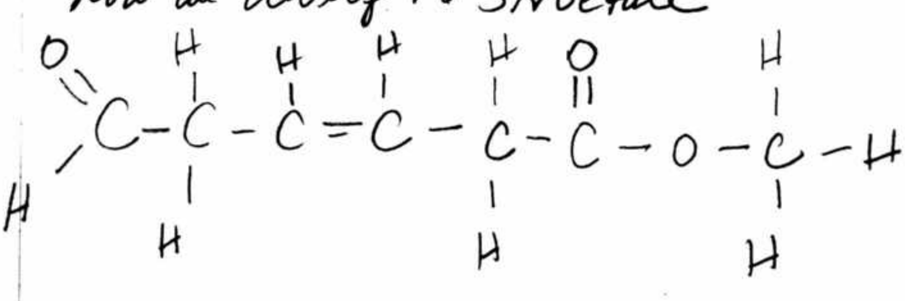
69% Ester



$-\overset{\overset{O}{\|}}{C}-O-C$

→ this causes a bend.

Now we develop the structure



Vitamin Cottage
Omega 3
Result w/ the Spreadsheet
- Identical