Code for analyzing EPR data

```
In[7]:= v := vt + vp
        nt := n0 ((vp / v) (tt / tp) + (vt / v)) ^ (-1)
        np := n0 ((vt / v) (tp / tt) + (vp / v)) ^ (-1)
        delnu := (1.1751 10 ^ (-2)) (4.52 + 0.00934 (tp - 273.150))
         polp := (shift / 2) / (delnu np)
        cal := sig / (polp nt)
```

Note, here "delnu" will be in (kHz/(amagat %))

September 27, 1998 – Don’t Worry – Nominal 100 C
Probably less than one hour wait time.
EPR fit done with Ioannis’s kumac. Don’t worry volumes should be considered preliminary.

```
In[13]:= n0 = 9.59
         vt= 94
         vp = 118
         tp = 102.9 + 273.15
         tt = 49.7 + 273.15
         shift = 16.3
         sig = 4.24
         cal

Out[13]= 9.59

Out[14]= 94

Out[15]= 118

Out[16]= 376.05

Out[17]= 322.85

Out[18]= 16.3

Out[19]= 4.24

Out[20]= 0.0287677
```

September 27, 1998 – Don’t Worry – Nominal 125 C
Wait was probably about an hour, maybe slightly more. EPR at 3:19AM.
EPR fits done with Ioannis’s kumac.

```
In[21]:= n0 = 9.59
         vt= 94
         vp = 118
         tp = 129.5 + 273.15
         tt = 51.8 + 273.15
         shift = 14.35
         sig = 4.11
         cal

Out[21]= 9.59

Out[22]= 94

Out[23]= 118

Out[24]= 402.65

Out[25]= 324.95

Out[26]= 14.35

Out[27]= 4.11

Out[28]= 0.0311245
```

September 27, 1998 – Don't Worry – Nominal 150 C
Wait was probably approaching two hours. EPR at 4:00AM.
EPR fits done with Ioannis's kumac.

```
In[29]:= n0 = 9.59
         vt= 94
         vp = 118
         tp = 154.5 + 273.15
         tt = 55.5 + 273.15
         shift = 13.84
         sig = 3.93
         cal

Out[29]= 9.59

Out[30]= 94

Out[31]= 118

Out[32]= 427.65

Out[33]= 328.65

Out[34]= 13.84

Out[35]= 3.93

Out[36]= 0.0305825
```

September 28, 1998 – Don't Worry – Nominal 120 C
Probably approaching two hours. EPR at 4:00AM
I fudged the temperatures because I cannot find an RTD printout.
EPR fit done with "ruler" method from plot.

```
In[37]:= n0 = 9.59
         vt= 94
         vp = 118
         tp = 124.5 + 273.15
         tt = 55.5 + 273.15
         shift = 21.1
         sig = 6.2
         cal

Out[37]= 9.59

Out[38]= 94

Out[39]= 118

Out[40]= 397.65

Out[41]= 328.65

Out[42]= 21.1

Out[43]= 6.2

Out[44]= 0.0324348
```

October 8, 1998 – Blue – Nominal 120 C
Very short waiting period, temperature down at 5:10PM, EPR at 5:37PM.
Not quite the usual sequence. There was one EPR first that I ignored
because it was not proceeded by an NMR measurement.
At the time I ran this I did not know Blue’s density, but for the calibration
constant alone that does not matter. I put in 19.59 to remind myself
to correct it later. EPR fit done with the "ruler" method.

```
In[45]:= n0 = 19.59
         vt= 94
         vp = 118
         tp = 125.5 + 273.15
         tt = 52.1 + 273.15
         shift = 12.81
         sig = 3.25
         cal

Out[45]= 19.59

Out[46]= 94

Out[47]= 118

Out[48]= 398.65

Out[49]= 325.25

Out[50]= 12.81

Out[51]= 3.25

Out[52]= 0.0276912
```

October 14, 1998 – Be Happy – Nominal 120 C
Be Happy volumes not yet calculated. I used the approximate Don’t Worry volumes.
This is the "stand–out" calibration. It was performed immediately following the
repair of the nmr coils, at a time when the NMR signal was dropping

fairly rapidly. The EPR was started at 4:08AM.
EPR fit was done using the "ruler" method.

```
In[53]:= n0 = 19.59
         vt= 94
         vp = 118
         tp = 122.1 + 273.15
         tt = 39.1 + 273.15
         shift = 21.6.81
         sig = 8.0
         cal

Out[53]= 19.59

Out[54]= 94

Out[55]= 118

Out[56]= 395.25

Out[57]= 312.25

Out[58]= 17.496

Out[59]= 8.

Out[60]= 0.0480546
```

October 15, 1998 – Be Happy – Nominal 175 C
My notes show the shift value of 31.1 kHz, I am not certain where
that came from. I also put a ruler on a plot generated by Carl's read–out kumac
and got 30.8 kHz.

```
In[61]:= n0 = 19.59
         vt= 94
         vp = 118
         tp = 187.3 + 273.15
         tt = 53.3 + 273.15
         shift = 30.8
         sig = 9.90
         cal

Out[61]= 19.59

Out[62]= 94

Out[63]= 118

Out[64]= 460.45

Out[65]= 326.45

Out[66]= 30.8

Out[67]= 9.9

Out[68]= 0.0335775
```

October 20, 1998 – Armegedon – Nominal 170 C
Armegedon volumes done carefully. Notes in my personal log.
I don't have any RTD printouts for the next four measurements, which were done

by Meme and Sebastien. I will include estimates only.
EPR fit is done using Ioannis's kumac.

```
In[69]:= n0 = 10.5
         vt= 87
         vp = 109.5
         v
         tp = 183 + 273.15
         tt = 50.0 + 273.15
         nt
         np
         shift = 34.3
         sig = 9.26
         polp
         cal

Out[69]= 10.5

Out[70]= 87

Out[71]= 109.5

Out[72]= 196.5

Out[73]= 456.15

Out[74]= 323.15

Out[75]= 12.537

Out[76]= 8.88157

Out[77]= 34.3

Out[78]= 9.26

Out[79]= 26.3795

Out[80]= 0.0279996
```

October 20, 1998 – Armegedon – Nominal 130 C
Oven changed to 130 at 9:22PM, and to 120 fat 9:36. EPR at 9:51. Thus, the wait is approaching but probably less than one half hour.
EPR fit done using Ioannis's kumac.

```
In[81]:= n0 = 10.5
         vt= 87
         vp = 109.5
         v = vt + vp
         tp = 133 + 273.15
         tt = 50.0 + 273.15
         nt
         np
         shift = 31.43
         sig = 8.385
         cal

Out[81]= 10.5

Out[82]= 87

Out[83]= 109.5

Out[84]= 196.5

Out[85]= 406.15

Out[86]= 323.15

Out[87]= 11.8494

Out[88]= 9.42788

Out[89]= 31.43

Out[90]= 8.385

Out[91]= 0.0287456
```

October 20, 1998 – Armegedon – Nominal 100 C
Oven changed to 100 at 9:56PM. EPR at 10:09. Wait is probably about one half hour.
EPR fit done using Ioannis's kumac.

```
In[92]:= n0 = 10.5
         vt= 87
         vp = 109.5
         v = vp + vt
         tp = 105 + 273.15
         tt = 45.0 + 273.15
         shift = 29.36
         sig = 8.115
         cal

Out[92]= 10.5

Out[93]= 87

Out[94]= 109.5

Out[95]= 196.5

Out[96]= 378.15

Out[97]= 318.15

Out[98]= 29.36

Out[99]= 8.115

Out[100]= 0.0300624
```

October 21, 1998 – Armegedon – Nominal 100 C
This taken after waiting about two hours. EPR at 12:09AM.
EPR fit done using Ioannis's kumac.

```
In[101]:= n0 = 19.59
          vt= 87
          vp = 109.5
          v = vt + vp
          tp = 105 + 273.15
          tt = 45.0 + 273.15
          shift = 26.8
          sig = 7.715
          cal

Out[101]= 19.59

Out[102]= 87

Out[103]= 109.5

Out[104]= 196.5

Out[105]= 378.15

Out[106]= 318.15

Out[107]= 26.8

Out[108]= 7.715

Out[109]= 0.0313106
```

October 22, 1998 – Armegedon – Nominal 170 C
EPR at 1:12PM. EPR fit done using ruler method.

```
n0 = 10.5
vt= 87
vp = 109.5
v = vt + vp
tp = 178 + 273.15
tt = 51.9 + 273.15
shift = 54.1
sig = 15.71
cal
```

```
Out[140]= 10.5

Out[141]= 87

Out[142]= 109.5

Out[143]= 196.5

Out[144]= 501.15

Out[145]= 325.05

Out[146]= 54.1

Out[147]= 15.71

Out[148]= 0.0294345
```

In this cell I will try understand the degree to which the lasers cause heating of the pumping cell beyond the set point of the oven. On October 25 we rotated the spins from transverse orientation to longitudinal orientation, and with longitudinal lasers off, measured the NMR signal to be 10.88mV. The RTD's read

RTD 1: 47.55	RTD 4: 52.44	RTD 7: 169.0
RTD 2: 50.41	RTD 5: 50.82	
RTD 3: 66.82	RTD 6: 163.88	

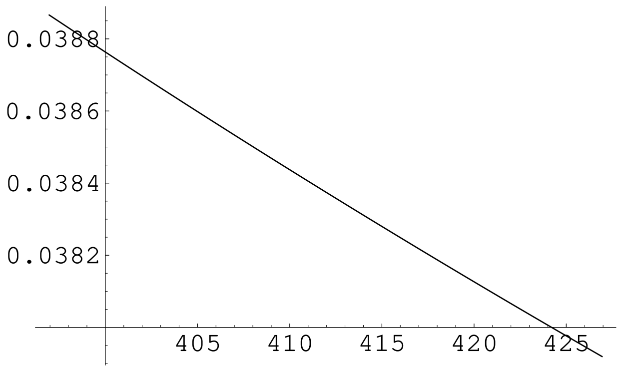
The oven set point during all of this was 170 C. In keeping with my proceedures above, I will average RTD's 1−5 for the lower cell temperature, and I will average RTD 7, RTD 8, and the oven setpoint as an estimate of the pumping cell temperature. This gives tt = 53.6, and tp = 167.6. After turning the lasers on, the NMR signal was 11.56mV. The RTD's read:

RTD 1: 47.4	RTD 4: 52.3	RTD 7: 178.8
RTD 2: 50.1	RTD 5: 50.6	
RTD 3: 67.2	RTD 6: 188.1	

```
In[119]:= n0 = 10.5
          vt= 87
          vp = 109.5
          v = vt + vp
          tp = 167.6 + 273.15
          tt = 53.6 + 273.15
          nt

Out[119]= 10.5

Out[120]= 87

Out[121]= 109.5

Out[122]= 196.5

Out[123]= 440.75

Out[124]= 326.75

Out[125]= 12.2683

In[137]:= FindRoot[13.0351 == nt, {tp, 453}]

Out[137]= {440.75 → 501.922}

In[138]:= tp = 501.992
          nt

Out[138]= 501.992

Out[139]= 13.0359
```

From the above numerical solution, it appears that the
pumping cell temperature needs to be fully 61 degrees hotter
than we computed to explain the rise in the NMR signal. My usual
way of computing the pumping cell temperature would yield 179 degrees.
Now 168 + 61 = 229. Thus, the indication is that the actual cell temperature
may be 50 degrees hotter than is indicated by my usual means of computing it.

```
Plot[cal, {tp, 123.8 + 273.15, 153.8 + 273.15}]
```



- Graphics -