THE ENTROPY OF LEAD

Computational Document

by

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The instructions for using this document are in the file cppbins.mcd.

The heat capacity data are located in a file called cplead. Values of Cp and absolute temperature are read into the computer. The computer then calculates values of ds = Cp/T for each temperature.

A := READPRN("CPLEAD.prn" ndata := rows(A) $i := 0 .. ndata - 1$

$T_i := \left(A^{<0>}\right)_i$ $Cp_i := \left(A^{<1>}\right)_i$ $dS_i := \frac{Cp_i}{T_i}$

This assigns the columns of the A matrix to temperature and heat capacity vectors.

Next view the contents of these vectors.

T =

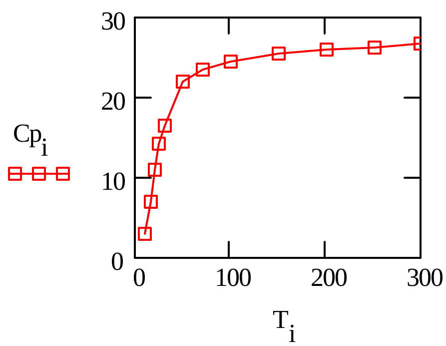
	0
0	10
1	15
2	20
3	25
4	30
5	50
6	70
7	100
8	150
9	200
10	250
11	298

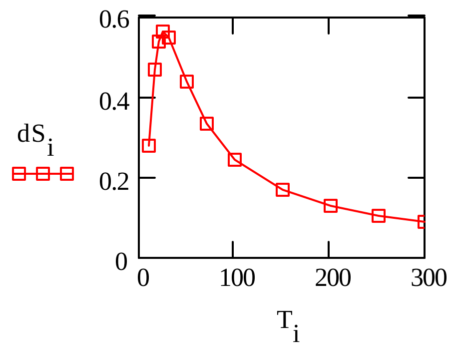
Cp =

	0
0	2.8
1	7
2	10.8
3	14.1
4	16.5
5	21.8
6	23.3
7	24.5
8	25.3
9	25.8
10	26.2
11	26.6

dS =

	0
0	0.28
1	0.467
2	0.54
3	0.564
4	0.55
5	0.436
6	0.333
7	0.245
8	0.169
9	0.129
10	0.105
11	0.089





To use the simple formula for trapezoid integration with evenly spaced points, we need to use interpolation methods. First we split up the space between the first and last points into N segments where we can adjust N.

$\Delta x := \frac{T_{ndata-1} - T_0}{N}$ $\quad j := 0 .. N \quad \Delta x = 28.8 \quad x_j := T_0 + j \cdot \Delta x$

The cspline function accumulates derivatives of the function at each point and puts them into a vector called vs.

$vs := cspline(T, dS)$

We can now find the value of the function at each x_j. On the graph below the black + signs are the experimental data, the red bars indicate the value of the function at evenly spaced points fx_j.

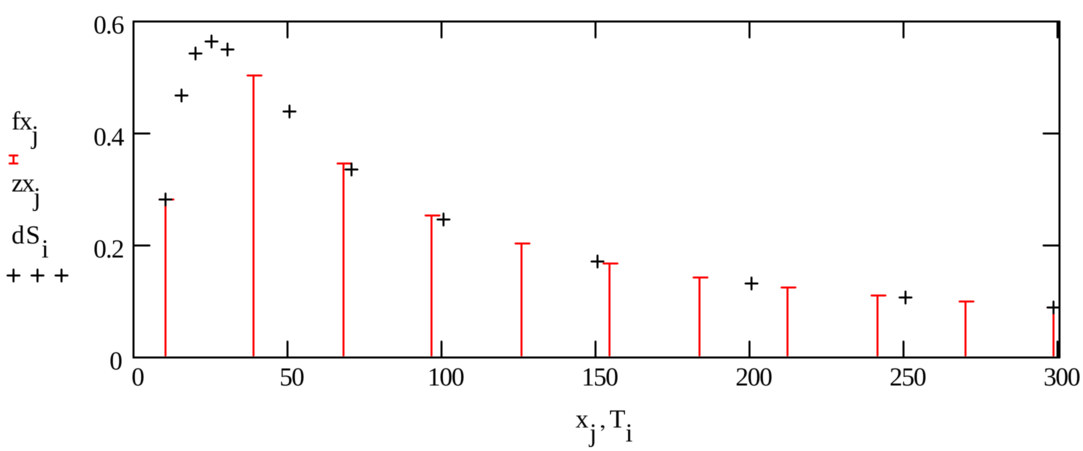
$fx_j := interp\left(vs, T, dS, x_j\right) \qquad zx_j := 0$

zx_j sets to lower level for the error bars.

$$Area := \sum_{j=1}^{N-1} \Delta x \cdot fx_j + \left[\frac{\left(fx_0 + fx_N\right)}{2} \cdot \Delta x\right]$$

The evenly spaced points are put into the area formula

$N \equiv 10 \qquad Area = 60.985$



Now we need to consider the contribution to the entropy for the region from 0º K up to the lowest temperature at which the heat capacity was measured T_0. In this region the heat capacity follows the function

$$Cp := a \cdot T^3 \qquad \frac{Cp}{T} := a \cdot T^2 \qquad \int_0^{T_0} \frac{Cp}{T} dT := \frac{Cp(T_0)}{3}$$

$Cp_0 = 2.8$

$$\Delta S := \frac{Cp_0}{3} \qquad \Delta S = 0.933$$

Therefore the total entropy for 0o K to 298o K is Area + ΔS

$$Area + \Delta S = 61.918$$