SIO 224 Homework 3

1a) What is the "Debye temperature" for a material? How is it determined and what is a typical value for mantle minerals?

1b) Given that the temperature in the deep mantle is well above the Debye temperature for candidate minerals, what do you expect the heat capacity (C_v or C_p) to be and how do you expect it to vary with temperature and pressure?

1c) In finite strain theory, there are two usual measures of strain: the Eulerian and Lagrangian. What is the difference between these two and which works best for practical applications and why?

2) The data on the next page are for the compression of magnesium silicate perovskite along a 300K isotherm. This is a compilation of four different experimental studies and two theoretical ab-initio studies (the latter are indicated by the asterixes and don't appear to be all that compatible with the experimental data – so you might want to consider fits without these – I have given them very large pressure errors so they should have little impact). (This table is available on the class web page.)

The volume at $P = 0$ is between 24.43 and 24.45 cm^3/mol. Do a finite strain(Eulerian) EOS fit to the data trying a 2nd, 3rd, and 4'th order fit. It is conventional to ignore the errors in the volume – and most mineral physicists ignore the errors in the pressure too (but don't you do this!). You should be able to compute formal uncertainties on your answers.

There are also other experimental constraints on K_{T0} from ultrasonics and Brillouin scattering. The latest of these give $K_{T0} = 251 \pm 5$GPa which you could use to constrain your fit.

How dependent are your answers on the finite strain equation used (in particular, how is the fit to the data impacted)?

Are there tradeoffs between parameters – does constraining the bulk modulus help?

What do you think of the ab-initio calculations?
PS – see additional notes on the class page to help you do this problem.

References:
1 Utsumi et al, 1995 V=24.43
2 Funamori et al, 1996 K'=4(assumed), K=261,
3 Fiquet et al, 1998 K'=4(assumed), K=256, V=24.46
4 Fiquet et al, 2000 K'=3.7, K=260, V=24.44
5 Saxena et al, 1999 K'=4(assumed), K=261, V=24.45
6 Organov et al, 2001 ab-initio
7 Li Li et al, 2005 ab-initio

Pressure(Gpa)	$\sigma_{Pressure}$	Vol (cm^3/mol)	Reference
4.60	.20	24.039	1
10.80	.20	23.455	1
13.80	.20	23.188	1
16.20	.20	23.026	1
16.60	.20	23.008	1
17.95	.20	22.929	1
20.00	.20	22.809	1
20.30	.20	22.803	1
23.10	.20	22.660	2
23.13	.20	22.669	2
23.28	.20	22.666	2
23.85	.20	22.573	2
26.53	.20	22.482	3
28.52	.20	22.217	3
29.50	.30	22.158	4
30.00	5.00	22.282	6*
31.47	.30	22.062	4
31.57	.30	22.066	4
36.20	.30	21.874	5
38.63	.30	21.646	4
39.44	.30	21.579	4
40.03	.30	21.596	4
40.66	.30	21.568	4
42.17	.30	21.467	4
43.17	.30	21.446	3
43.48	.30	21.413	3
45.11	.20	21.356	3
45.38	.30	21.278	4
45.90	.30	21.343	3
46.44	.30	21.258	4
46.88	.30	21.202	4
47.49	.30	21.206	3
48.33	.30	21.200	3
49.51	.30	21.178	3
49.59	.30	21.154	3
49.59	.30	21.195	3
50.94	.30	21.049	4
53.46	.30	20.973	4
53.63	.30	20.968	4
53.80	.30	20.995	5
54.33	.30	20.922	3
60.00	5.00	20.792	6*
60.10	.30	20.717	5
65.50	.30	20.491	5
65.88	.30	20.334	4
67.50	.30	20.410	5
67.94	.30	20.295	4
70.12	.30	20.120	4
71.50	.30	20.114	4
75.06	.30	19.983	4
75.62	.30	19.992	4
77.60	.30	20.022	5
78.60	.30	19.986	5
80.10	.30	19.930	5
80.57	.30	19.821	4
82.20	.30	19.857	5
82.50	.30	19.846	5
85.32	.30	19.612	4
85.70	.30	19.587	4
90.00	5.00	19.662	6*
90.17	.30	19.467	4
90.57	.30	19.465	4
120.00	5.00	18.743	6*
142.00	5.00	18.05	7*
150.00	5.00	17.99	6*