

Output

Axes	K(TPa ⁻¹)	σ_K (TPa ⁻¹)	Direction			Empirical parameters			P_c	ν
			a	b	c	ϵ_0	λ			
X₁	8.1616	0.2327	0.7071	-0.7071	0.0000	5.3078e-04	-9.0847e-03		0.0000	0.9136
X₂	8.1616	0.2327	-0.7071	-0.7071	0.0000	5.3078e-04	-9.0847e-03		0.0000	0.9136
X₃	8.1616	0.2327	0.0000	0.0000	1.0000	5.3078e-04	-9.0847e-03		0.0000	0.9136
V	24.9232	0.5975								

Birch-Murnaghan Coefficients

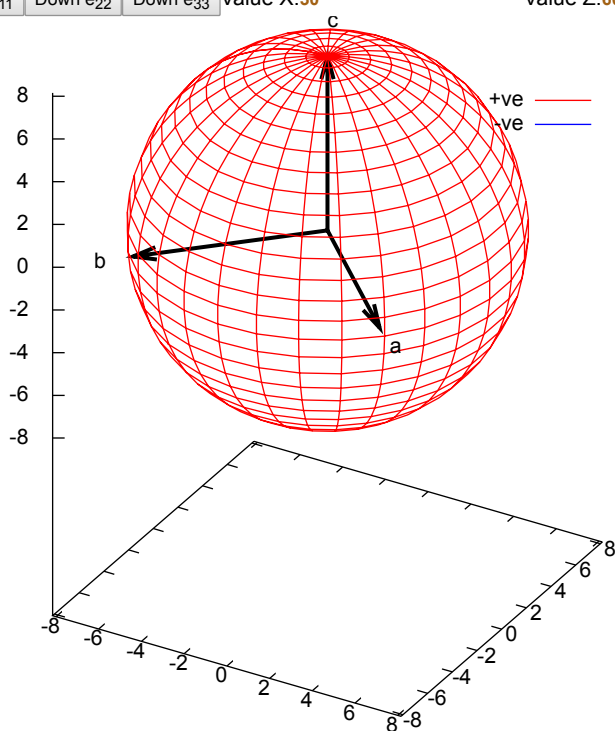
	B_0 (GPa)	σB_0 (GPa)	V_0 (Å ³)	σV_0 (Å ³)	B'	$\sigma B'$	P_c (GPa)
2nd	35.1816	0.6236	14953.6843	8.2862	4	n/a	0
3rd	31.1918	2.5250	14970.8234	14.5098	8.3638	2.8834	0

Compressibility Indicatrix

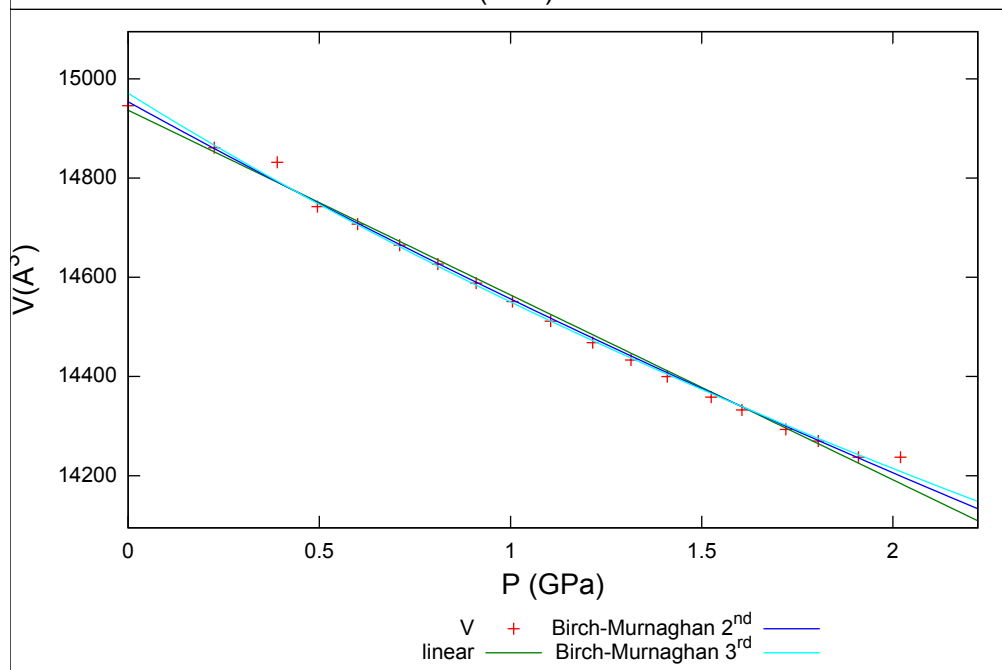
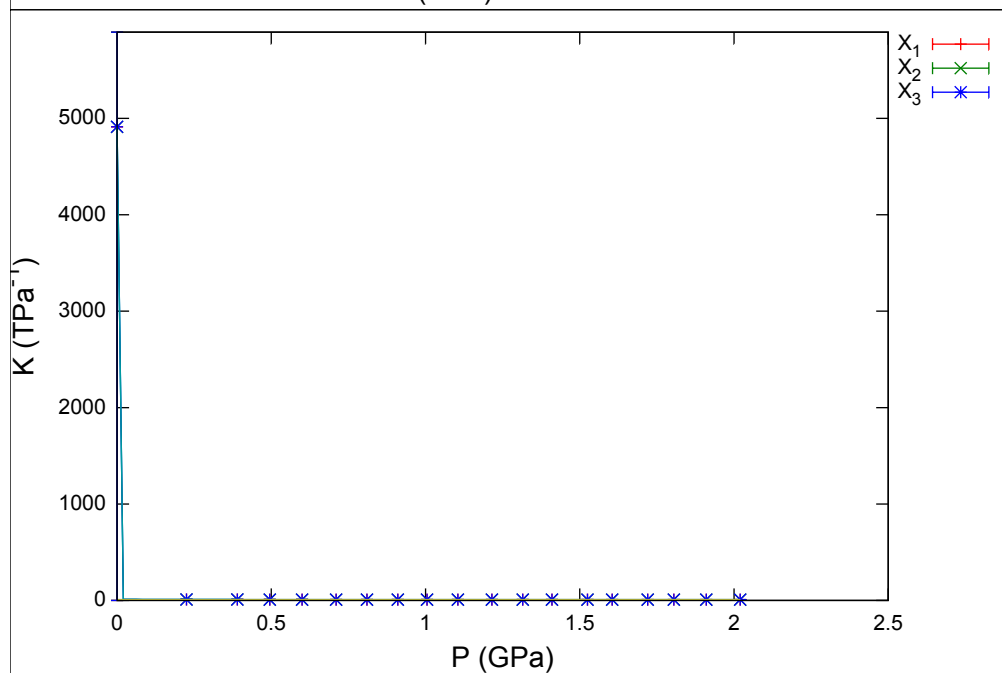
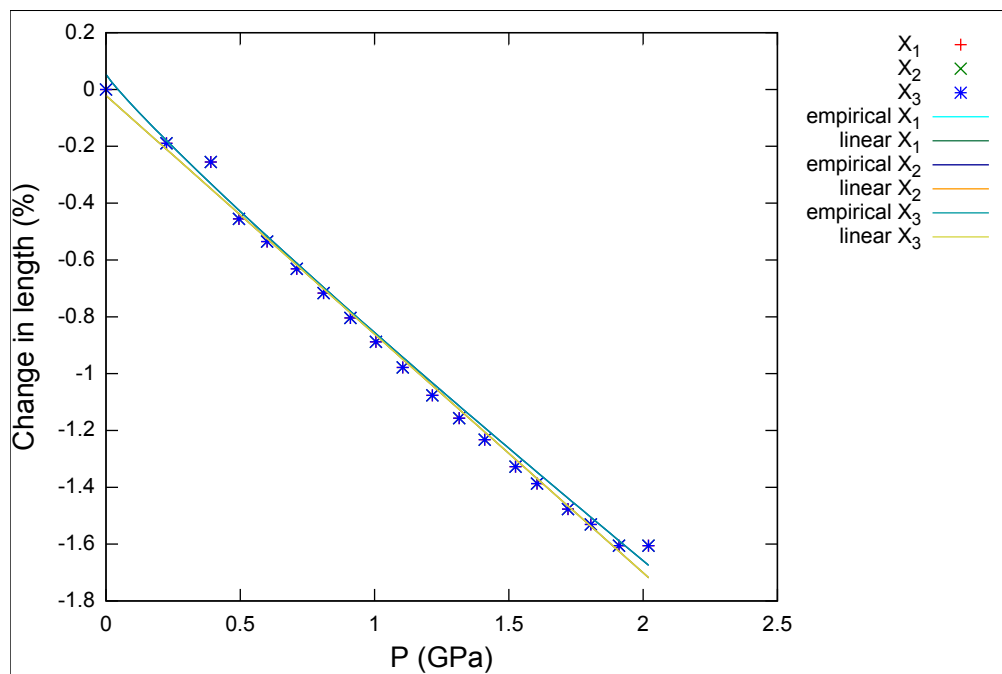
The compressibility indicatrix has units of TPa⁻¹.

Rotate +x	Rotate -x	Rotate +z	Rotate -z
Down e ₁₁	Down e ₂₂	Down e ₃₃	Value X:30

Value Z:60



Plots



Compressibilities (TPa⁻¹)

2/9/2018				PASCAL			
P	K ₁	K ₂	K ₃	σK ₁	σK ₂	σK ₃	
0.00	4911.90	4911.90	4911.91	10618568760686593623839960203264.00	10618568760686593623839960203264.00	10618571353299112601118285	
0.23	9.44	9.44	9.44	1.34	1.34	1.34	
0.39	9.00	9.00	9.00	0.83	0.83	0.83	
0.49	8.82	8.82	8.82	0.63	0.63	0.63	
0.60	8.67	8.67	8.67	0.48	0.48	0.48	
0.71	8.55	8.55	8.55	0.36	0.36	0.36	
0.81	8.45	8.45	8.45	0.27	0.27	0.27	
0.91	8.37	8.37	8.37	0.22	0.22	0.22	
1.00	8.30	8.30	8.30	0.20	0.20	0.20	
1.10	8.23	8.23	8.23	0.20	0.20	0.20	
1.22	8.16	8.16	8.16	0.23	0.23	0.23	
1.31	8.11	8.11	8.11	0.27	0.27	0.27	
1.41	8.06	8.06	8.06	0.30	0.30	0.30	
1.52	8.00	8.00	8.00	0.35	0.35	0.35	
1.60	7.97	7.97	7.97	0.38	0.38	0.38	
1.72	7.92	7.92	7.92	0.42	0.42	0.42	
1.80	7.89	7.89	7.89	0.45	0.45	0.45	
1.91	7.85	7.85	7.85	0.49	0.49	0.49	
2.02	7.81	7.81	7.81	0.52	0.52	0.52	

% change in length

P	X ₁	X ₂	X ₃	X _{1,calc}	X _{2,calc}	X _{3,calc}
0.0000	0.0000	0.0000	0.0000	0.0531	0.0531	0.0531
0.2250	-0.1894	-0.1894	-0.1894	-0.1794	-0.1794	-0.1794
0.3900	-0.2551	-0.2551	-0.2551	-0.3312	-0.3312	-0.3312
0.4950	-0.4554	-0.4554	-0.4554	-0.4248	-0.4248	-0.4248
0.6000	-0.5351	-0.5351	-0.5351	-0.5166	-0.5166	-0.5166
0.7100	-0.6311	-0.6311	-0.6311	-0.6113	-0.6113	-0.6113
0.8100	-0.7168	-0.7168	-0.7168	-0.6963	-0.6963	-0.6963
0.9100	-0.8039	-0.8039	-0.8039	-0.7804	-0.7804	-0.7804
1.0050	-0.8880	-0.8880	-0.8880	-0.8595	-0.8595	-0.8595
1.1050	-0.9781	-0.9781	-0.9781	-0.9422	-0.9422	-0.9422
1.2150	-1.0765	-1.0765	-1.0765	-1.0323	-1.0323	-1.0323
1.3150	-1.1566	-1.1566	-1.1566	-1.1136	-1.1136	-1.1136
1.4100	-1.2325	-1.2325	-1.2325	-1.1904	-1.1904	-1.1904
1.5250	-1.3273	-1.3273	-1.3273	-1.2828	-1.2828	-1.2828
1.6050	-1.3868	-1.3868	-1.3868	-1.3466	-1.3466	-1.3466
1.7200	-1.4768	-1.4768	-1.4768	-1.4380	-1.4380	-1.4380
1.8050	-1.5309	-1.5309	-1.5309	-1.5052	-1.5052	-1.5052
1.9100	-1.6057	-1.6057	-1.6057	-1.5878	-1.5878	-1.5878
2.0200	-1.6057	-1.6057	-1.6057	-1.6739	-1.6739	-1.6739

Volume

P	P _{lin}	P _{calc,2nd}	P _{3rd}	V (Å ³)
0.0000	-0.0241	0.0187	0.0527	14945.7313
0.2250	0.2035	0.2216	0.2369	14860.9643
0.3900	0.2822	0.2931	0.3029	14831.6488
0.4950	0.5216	0.5149	0.5111	14742.4616
0.6000	0.6165	0.6048	0.5968	14707.0992
0.7100	0.7307	0.7142	0.7024	14664.5597
0.8100	0.8325	0.8132	0.7989	14626.6359
0.9100	0.9358	0.9149	0.8991	14588.1560
1.0050	1.0353	1.0141	0.9978	14551.0882
1.1050	1.1418	1.1215	1.1057	14511.4523
1.2150	1.2578	1.2403	1.2264	14468.2437
1.3150	1.3521	1.3382	1.3268	14433.1079
1.4100	1.4412	1.4318	1.4236	14399.8935
1.5250	1.5524	1.5500	1.5470	14358.4768
1.6050	1.6222	1.6249	1.6260	14332.4935
1.7200	1.7274	1.7393	1.7474	14293.3105
1.8050	1.7906	1.8087	1.8217	14269.7708
1.9100	1.8778	1.9054	1.9259	14237.2974
2.0200	1.8778	1.9054	1.9259	14237.2904

Input

P σP a b c α β γ

0	0.1	24.632343	24.632343	24.632343	90	90	90
0.225	0.1	24.585686	24.585686	24.585686	90	90	90
0.39	0.1	24.569509	24.569509	24.569509	90	90	90
0.495	0.1	24.520162	24.520162	24.520162	90	90	90
0.6	0.1	24.500541	24.500541	24.500541	90	90	90
0.71	0.1	24.476896	24.476896	24.476896	90	90	90
0.81	0.1	24.455778	24.455778	24.455778	90	90	90
0.91	0.1	24.434313	24.434313	24.434313	90	90	90
1.005	0.1	24.4136	24.4136	24.4136	90	90	90
1.105	0.1	24.391413	24.391413	24.391413	90	90	90
1.215	0.1	24.36718	24.36718	24.36718	90	90	90
1.315	0.1	24.347439	24.347439	24.347439	90	90	90
1.41	0.1	24.328748	24.328748	24.328748	90	90	90
1.525	0.1	24.305401	24.305401	24.305401	90	90	90
1.605	0.1	24.290731	24.290731	24.290731	90	90	90
1.72	0.1	24.268575	24.268575	24.268575	90	90	90
1.805	0.1	24.255245	24.255245	24.255245	90	90	90
1.91	0.1	24.236832	24.236832	24.236832	90	90	90
2.02	0.1	24.236828	24.236828	24.236828	90	90	90