

Output

Axes			Direction			Empirical parameters				P_c	ν
	$K(\text{TPa}^{-1})$	$\sigma K(\text{TPa}^{-1})$	a	b	c	ϵ_0	λ				
X_1	7.9499	0.1452	0.0000	0.0000	1.0000	-2.9826e-05	-8.2506e-03			0.0000	0.9568
X_2	7.9902	0.1231	-0.3620	-0.9322	0.0000	-1.1988e-04	-7.8479e-03			0.0000	1.0217
X_3	5.6374	0.3162	-0.9905	-0.1373	0.0000	5.8430e-04	-8.0668e-03			0.0000	0.6614
V	21.8337	0.4509									

Birch-Murnaghan Coefficients

	B_0 (GPa)	σB_0 (GPa)	V_0 ($\text{\AA}^3$)	σV_0 ($\text{\AA}^3$)	B'	$\sigma B'$	P_c (GPa)
2 nd	41.1095	0.8220	7418.3463	3.6169	4	n/a	0
3 rd	37.4147	2.9232	7421.8778	4.8068	8.2688	3.4738	0

Compressibility Indicatrix

The compressibility indicatrix has units of TPa^{-1} .

Rotate +x

Rotate -x

Rotate +z

Rotate -z

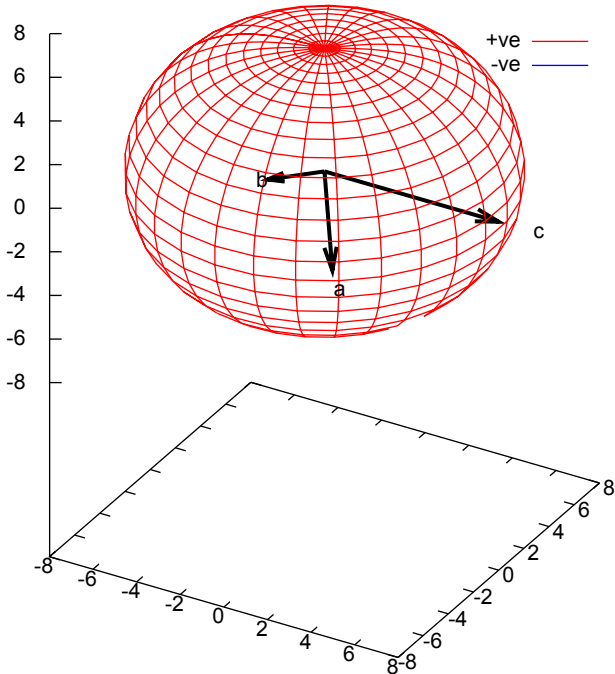
Down e_{11}

Down e_{22}

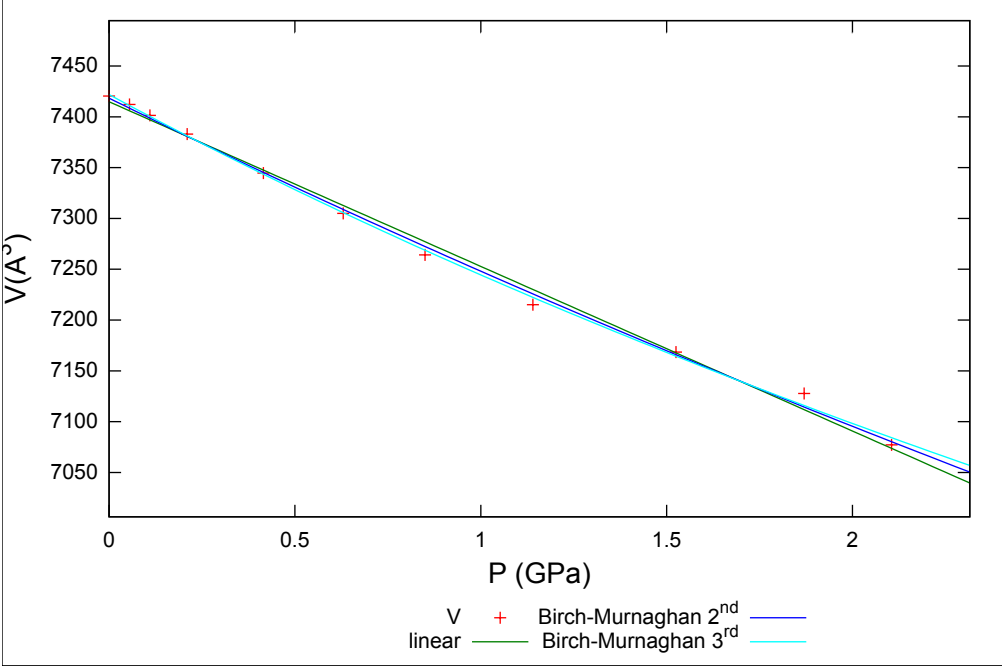
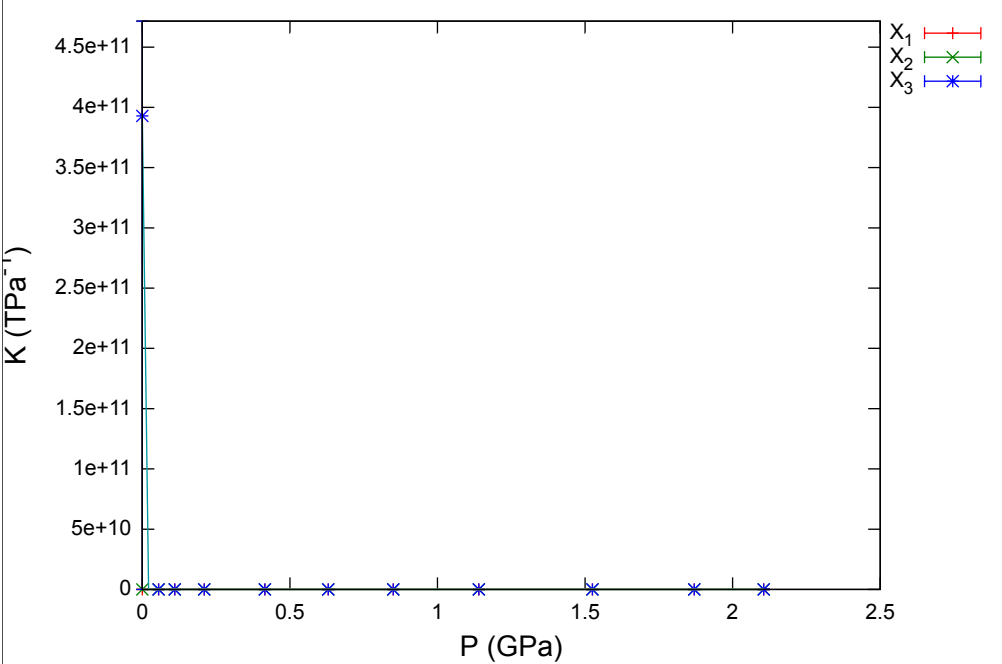
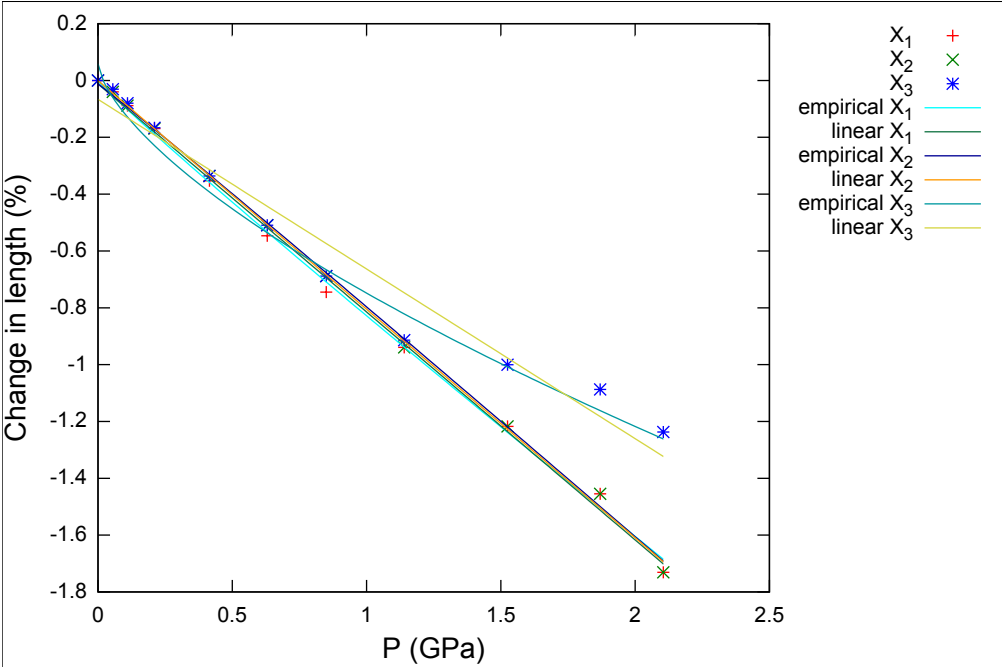
Down e_{33}

Value X:**30**

Value Z:**60**



Plots



Compressibilities (TPa⁻¹)

P	K ₁	K ₂	K ₃	σK_1	σK_2	σK_3
0.00	192.20	1.61	392963159321.49	2530500746232216296521381969920.00	266871263509864263129071878144.00	511858479572141195050716
0.06	8.95	7.53	14.24	1.29	0.89	4.53
0.11	8.68	7.64	11.27	0.94	0.71	2.63
0.21	8.44	7.75	9.05	0.64	0.51	1.42
0.41	8.20	7.87	7.19	0.34	0.30	0.59
0.63	8.05	7.94	6.24	0.19	0.17	0.33
0.85	7.95	7.99	5.64	0.15	0.12	0.32
1.14	7.85	8.04	5.10	0.19	0.15	0.40
1.52	7.75	8.09	4.63	0.28	0.23	0.50
1.87	7.68	8.13	4.32	0.35	0.30	0.57
2.10	7.64	8.15	4.15	0.39	0.34	0.60

% 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	-0.0030	-0.0120	0.0584
0.0550	-0.0403	-0.0403	-0.0305	-0.0544	-0.0525	-0.0600
0.1100	-0.0883	-0.0883	-0.0799	-0.1028	-0.0943	-0.1289
0.2100	-0.1694	-0.1694	-0.1666	-0.1883	-0.1713	-0.2289
0.4150	-0.3528	-0.3363	-0.3363	-0.3586	-0.3315	-0.3925
0.6300	-0.5466	-0.5093	-0.5093	-0.5333	-0.5015	-0.5358
0.8500	-0.7447	-0.6886	-0.6886	-0.7092	-0.6767	-0.6660
1.1400	-0.9391	-0.9391	-0.9141	-0.9382	-0.9092	-0.8213
1.5250	-1.2175	-1.2175	-1.0002	-1.2385	-1.2198	-1.0080
1.8700	-1.4549	-1.4549	-1.0873	-1.5047	-1.4997	-1.1620
2.1050	-1.7310	-1.7310	-1.2370	-1.6848	-1.6909	-1.2614

Volume

P	P _{lin}	P _{calc,2nd}	P _{3rd}	V (Å ³)
0.0000	-0.0349	-0.0117	0.0072	7420.4501
0.0550	0.0160	0.0341	0.0490	7412.2131
0.1100	0.0825	0.0943	0.1044	7401.4313
0.2100	0.1963	0.1982	0.2008	7383.0027
0.4150	0.4331	0.4189	0.4087	7344.6260
0.6300	0.6783	0.6533	0.6345	7304.9052
0.8500	0.9301	0.9008	0.8780	7264.1089
1.1400	1.2322	1.2069	1.1864	7215.1627
1.5250	1.5206	1.5087	1.4980	7168.4444
1.8700	1.7717	1.7795	1.7839	7127.7475
2.1050	2.0841	2.1269	2.1591	7077.1381

Input

P	σP	a	b	c	α	β	γ
0	0.1	17.38193	17.38193	28.35983	90	90	120
0.055	0.1	17.37493	17.37493	28.35118	90	90	120
0.11	0.1	17.36658	17.36658	28.33717	90	90	120
0.21	0.1	17.35248	17.35248	28.31257	90	90	120
0.415	0.1	17.32348	17.32348	28.25978	90	90	120
0.63	0.1	17.2934	17.2934	28.20481	90	90	120
0.85	0.1	17.26224	17.26224	28.14864	90	90	120
1.14	0.1	17.21869	17.21869	28.10058	90	90	120
1.525	0.1	17.17031	17.17031	28.07618	90	90	120
1.87	0.1	17.12904	17.12904	28.05147	90	90	120
2.105	0.1	17.08105	17.08105	28.00902	90	90	120