

Output

Axes	Direction			Empirical parameters					
	$K(\text{TPa}^{-1})$	$\sigma K(\text{TPa}^{-1})$	a	b	c	ϵ_0	λ	P_c	ν
X_1	12.4917	0.3726	0.0000	1.0000	-0.0000	9.2025e-04	-1.2126e-02	0.2750	1.0272
X_2	12.4917	0.3726	1.0000	-0.0000	-0.0000	9.2024e-04	-1.2126e-02	0.2750	1.0272
X_3	12.4917	0.3725	0.0000	0.0000	1.0000	9.2032e-04	-1.2126e-02	0.2750	1.0272
V	36.8399	0.8430							

Birch-Murnaghan Coefficients

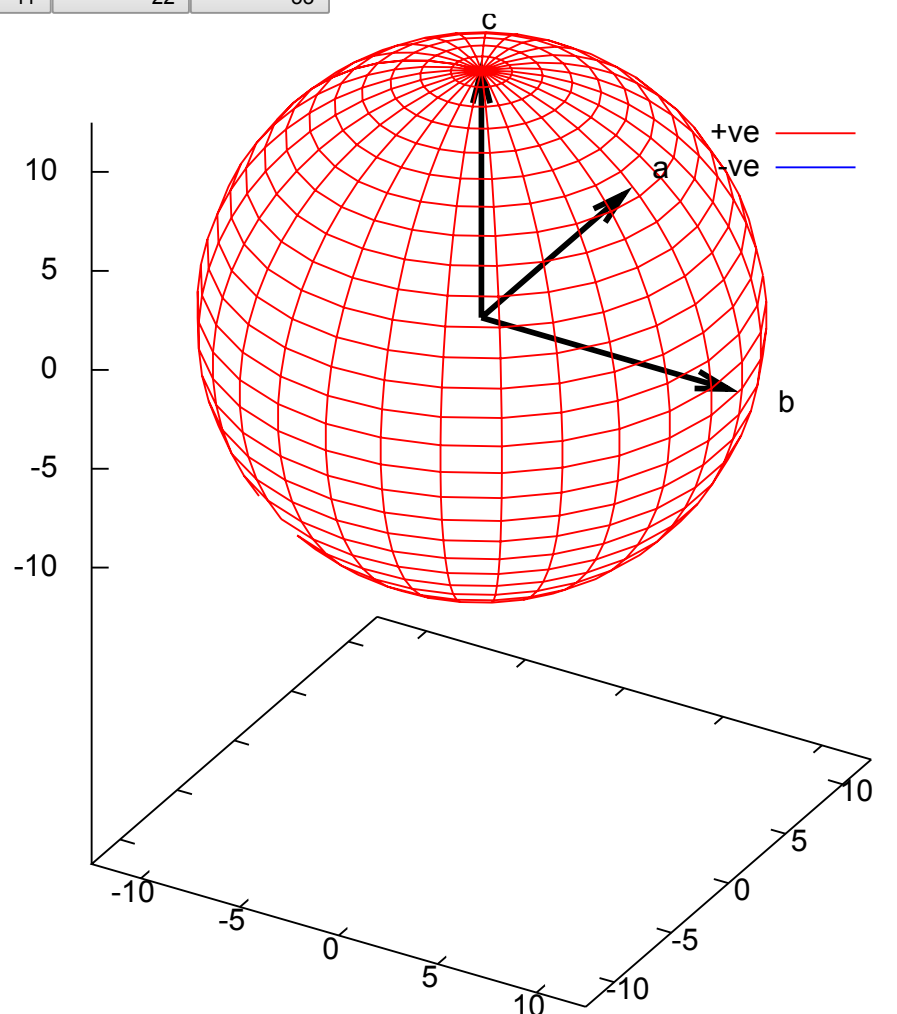
	B_0 (GPa)	σB_0 (GPa)	V_0 (\AA^3)	σV_0 (\AA^3)	B'	$\sigma B'$	P_c (GPa)
2 nd	21.6151	0.5115	3140.8709	3.7844	4	n/a	0
3 rd	22.7735	2.7163	3137.7213	7.9152	3.0350	2.1580	0

Compressibility Indicatrix

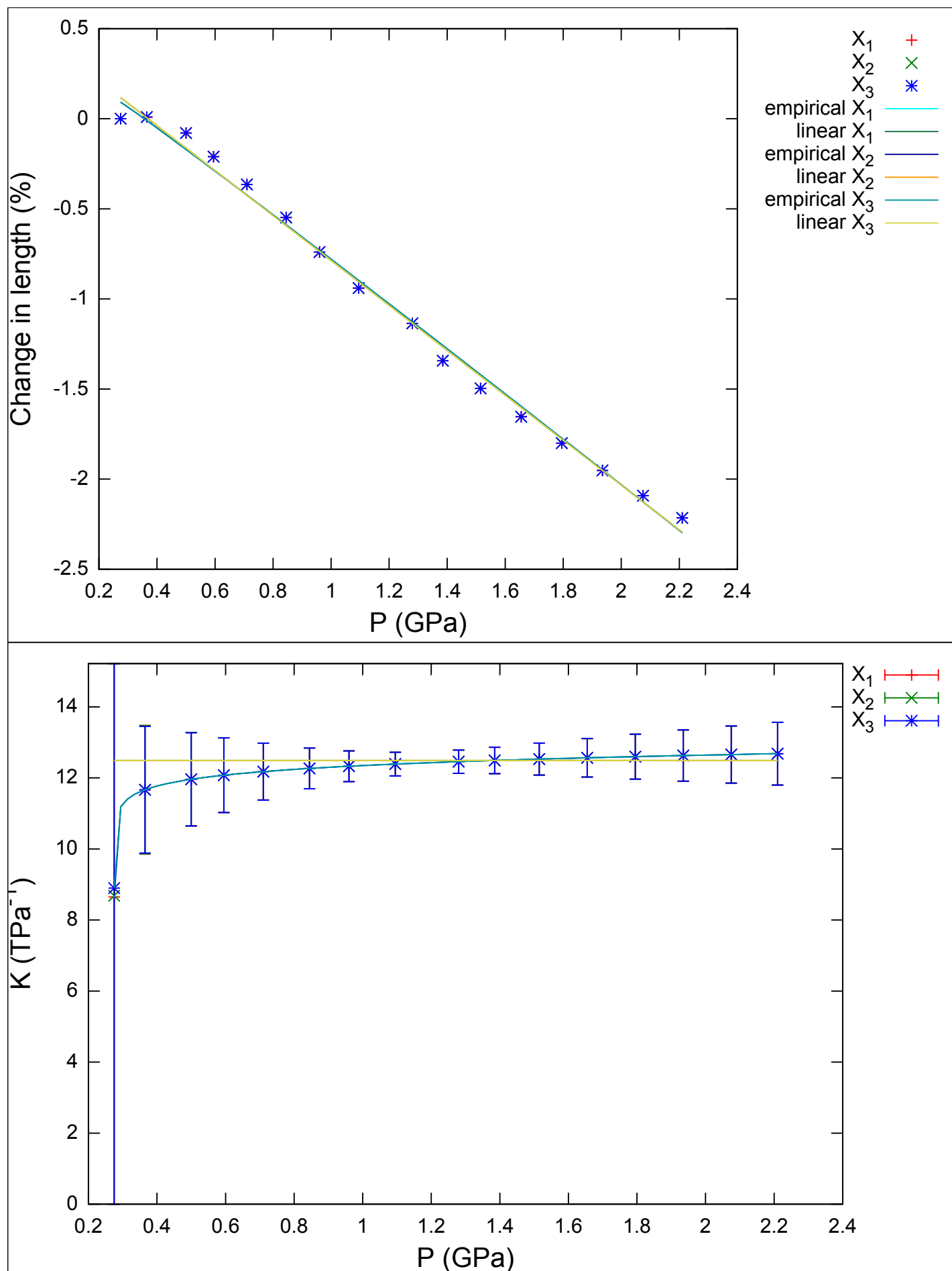
The compressibility indicatrix has units of TPa^{-1} .

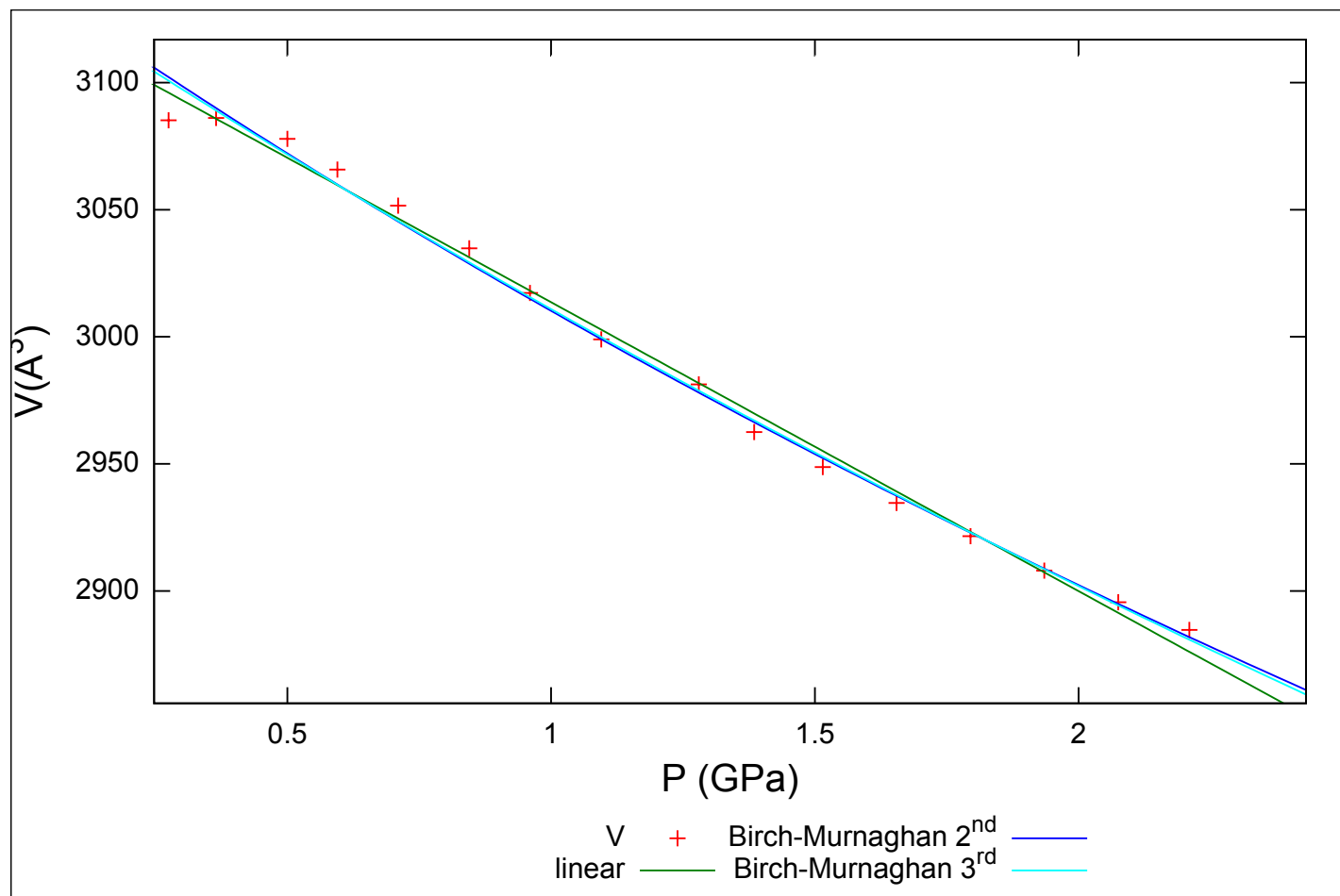
Rotate +x	Rotate -x	Rotate +z	Rotate -z
Down e_{11}	Down e_{22}	Down e_{33}	Value X:30

Value Z:60



Plots





Compressibilities (TPa⁻¹)

P	K ₁	K ₂	K ₃	σK ₁	σK ₂	σK ₃
0.28	8.65	8.68	8.90	54580.48	47242.97	21569.89
0.36	11.67	11.67	11.67	1.81	1.81	1.78
0.50	11.96	11.96	11.96	1.32	1.32	1.31
0.59	12.08	12.08	12.08	1.05	1.05	1.05
0.71	12.18	12.18	12.18	0.80	0.80	0.80
0.84	12.27	12.27	12.27	0.57	0.57	0.58
0.96	12.33	12.33	12.33	0.43	0.43	0.43
1.09	12.39	12.39	12.39	0.33	0.33	0.33
1.28	12.46	12.46	12.46	0.33	0.33	0.33
1.39	12.49	12.49	12.49	0.37	0.37	0.37
1.51	12.53	12.53	12.53	0.45	0.45	0.45
1.66	12.57	12.57	12.57	0.54	0.54	0.54
1.79	12.60	12.60	12.60	0.63	0.63	0.63
1.94	12.63	12.63	12.63	0.72	0.72	0.72
2.08	12.66	12.66	12.66	0.80	0.80	0.81
2.21	12.68	12.68	12.68	0.88	0.88	0.88

% change in length

P	X ₁	X ₂	X ₃	X _{1,calc}	X _{2,calc}	X _{3,calc}
0.2750	0.0000	0.0000	0.0000	0.0920	0.0920	0.0920
0.3650	0.0094	0.0094	0.0094	-0.0102	-0.0102	-0.0102
0.5000	-0.0794	-0.0794	-0.0794	-0.1700	-0.1700	-0.1700

0.5950 -0.2101 -0.2101 -0.2101 -0.2842 -0.2842 -0.2842
 0.7100 -0.3643 -0.3643 -0.3643 -0.4237 -0.4237 -0.4237
 0.8450 -0.5478 -0.5478 -0.5478 -0.5887 -0.5887 -0.5887
 0.9600 -0.7399 -0.7399 -0.7399 -0.7301 -0.7301 -0.7301
 1.0950 -0.9399 -0.9399 -0.9399 -0.8970 -0.8970 -0.8970
 1.2800 -1.1359 -1.1359 -1.1359 -1.1268 -1.1268 -1.1268
 1.3850 -1.3431 -1.3431 -1.3431 -1.2578 -1.2578 -1.2578
 1.5150 -1.4965 -1.4965 -1.4965 -1.4205 -1.4205 -1.4205
 1.6550 -1.6535 -1.6535 -1.6535 -1.5961 -1.5961 -1.5961
 1.7950 -1.8004 -1.8004 -1.8004 -1.7723 -1.7723 -1.7723
 1.9350 -1.9521 -1.9521 -1.9521 -1.9489 -1.9489 -1.9489
 2.0750 -2.0917 -2.0917 -2.0917 -2.1259 -2.1259 -2.1259
 2.2100 -2.2152 -2.2152 -2.2152 -2.2969 -2.2969 -2.2969

Volume

P	P _{lin}	P _{calc,2nd}	P _{3rd}	V (Å ³)
0.2750	0.3701	0.4008	0.3945	3085.1815
0.3650	0.3625	0.3942	0.3878	3086.0519
0.5000	0.4347	0.4563	0.4518	3077.8389
0.5950	0.5409	0.5490	0.5471	3065.7750
0.7100	0.6658	0.6604	0.6612	3051.5816
0.8450	0.8138	0.7957	0.7990	3034.7614
0.9600	0.9682	0.9409	0.9461	3017.2093
1.0950	1.1284	1.0959	1.1023	2999.0012
1.2800	1.2847	1.2515	1.2582	2981.2376
1.3850	1.4493	1.4203	1.4264	2962.5292
1.5150	1.5707	1.5482	1.5530	2948.7337
1.6550	1.6945	1.6815	1.6845	2934.6582
1.7950	1.8100	1.8088	1.8094	2921.5263
1.9350	1.9289	1.9426	1.9401	2908.0119
2.0750	2.0381	2.0681	2.0622	2895.6002
2.2100	2.1344	2.1809	2.1715	2884.6571

Input

P	σP	a	b	c	α	β	γ
0.275	0.1	14.557727	14.557727	14.557727	90	90	90
0.365	0.1	14.559096	14.559096	14.559096	90	90	90
0.5	0.1	14.546169	14.546169	14.546169	90	90	90
0.595	0.1	14.527139	14.527139	14.527139	90	90	90
0.71	0.1	14.504686	14.504686	14.504686	90	90	90
0.845	0.1	14.477987	14.477987	14.477987	90	90	90
0.96	0.1	14.450021	14.450021	14.450021	90	90	90
1.095	0.1	14.420895	14.420895	14.420895	90	90	90
1.28	0.1	14.392366	14.392366	14.392366	90	90	90
1.385	0.1	14.362197	14.362197	14.362197	90	90	90
1.515	0.1	14.339869	14.339869	14.339869	90	90	90
1.655	0.1	14.317016	14.317016	14.317016	90	90	90
1.795	0.1	14.295629	14.295629	14.295629	90	90	90

1.935	0.1	14.273552	14.273552	14.273552	90	90	90
2.075	0.1	14.253216	14.253216	14.253216	90	90	90
2.21	0.1	14.235238	14.235238	14.235238	90	90	90