

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	8.0448	0.1721	1.0000	-0.0000	-0.0000	-2.0342e-04	-6.8462e-03	0.0000 1.2346
X_2	8.0448	0.1721	0.0000	1.0000	-0.0000	-2.0342e-04	-6.8462e-03	0.0000 1.2346
X_3	8.0448	0.1721	0.0000	0.0000	1.0000	-2.0342e-04	-6.8462e-03	0.0000 1.2346
V	21.9887	0.6875						

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	41.9470	1.4166	6527.0277	3.8453	4	n/a	0
3 rd	57.2987	0.9354	6517.0390	0.7338	-13.9804	0.8692	0

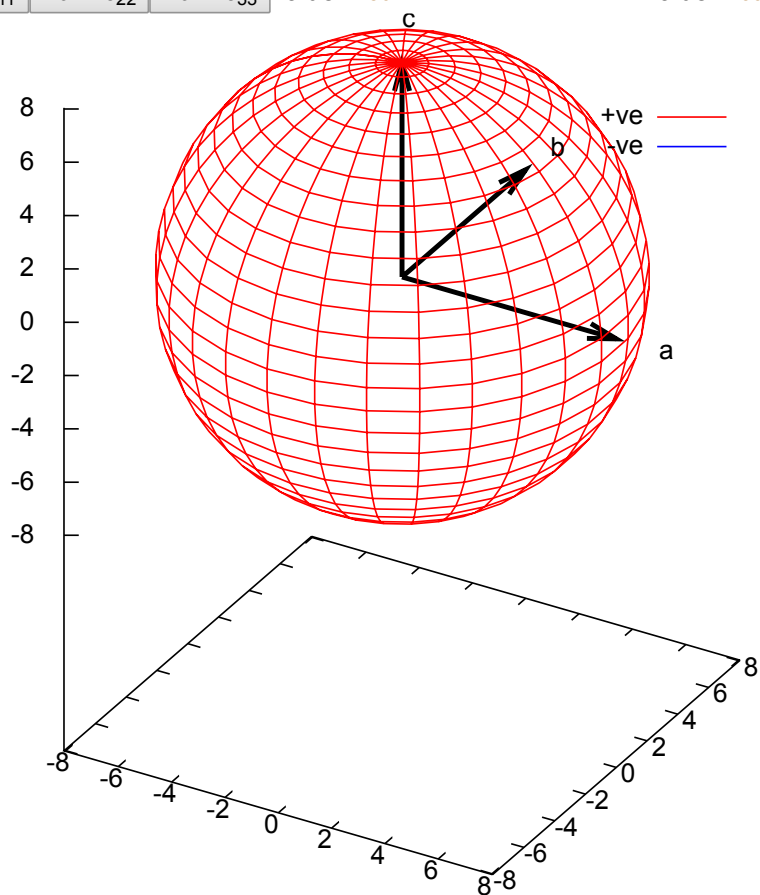
Compressibility Indicatrix

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

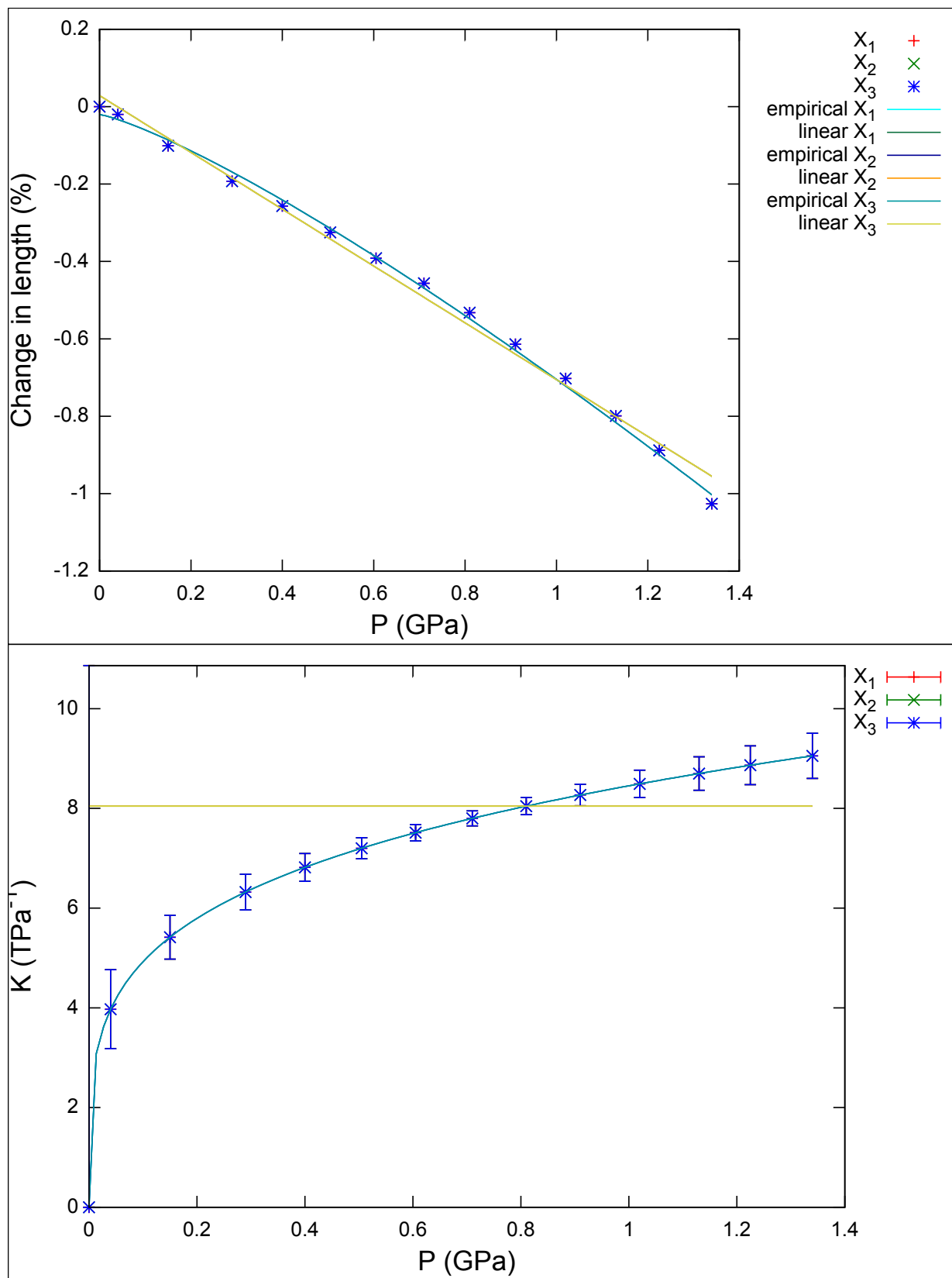
Rotate +x	Rotate -x	Rotate +z	Rotate -z
Down e_{11}	Down e_{22}	Down e_{33}	

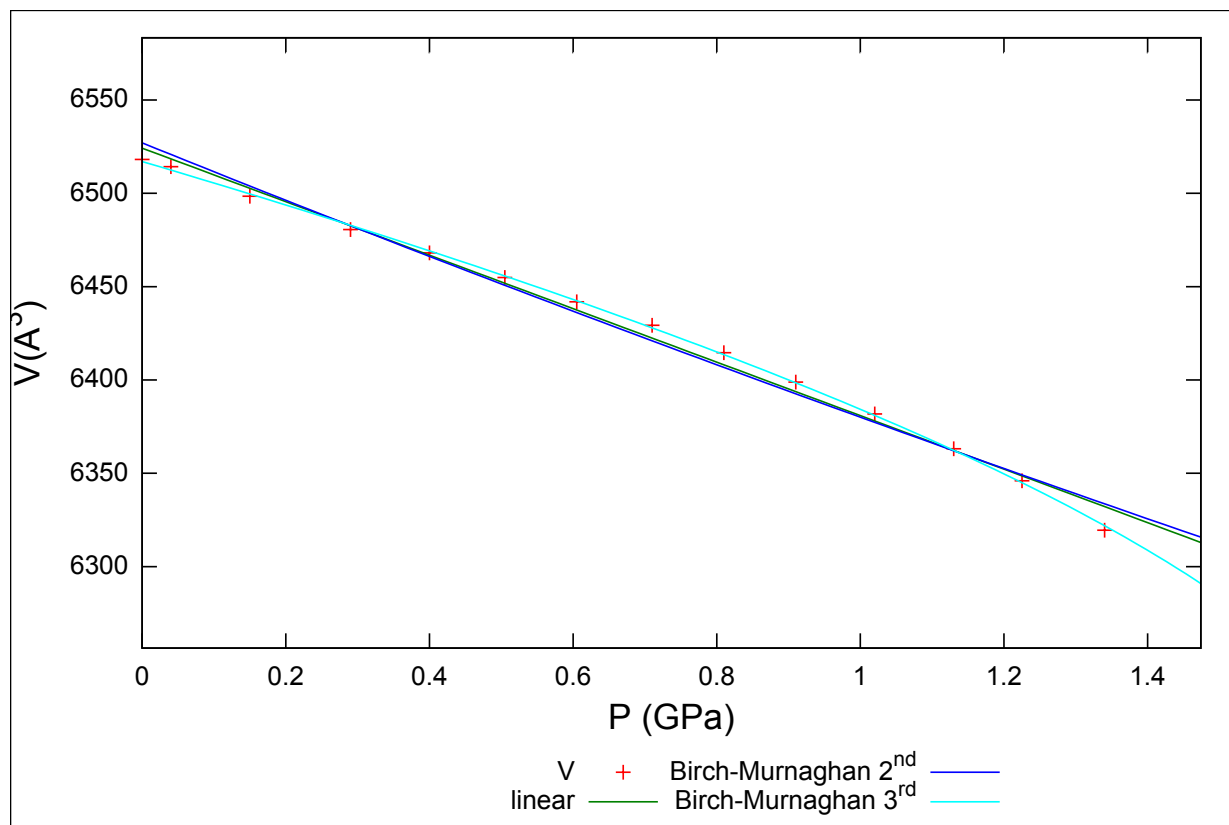
Value X:30

Value Z:60



Plots





Compressibilities (TPa⁻¹)

P	K ₁	K ₂	K ₃	σK ₁	σK ₂	σK ₃
0.00	0.00	0.00	0.00	462500513398386707136512.00	462500513398386707136512.00	462500180515980935430144.00
0.04	3.97	3.97	3.97	0.79	0.79	0.79
0.15	5.42	5.42	5.42	0.44	0.44	0.44
0.29	6.32	6.32	6.32	0.36	0.36	0.36
0.40	6.82	6.82	6.82	0.28	0.28	0.28
0.51	7.20	7.20	7.20	0.21	0.21	0.21
0.60	7.51	7.51	7.51	0.17	0.17	0.17
0.71	7.80	7.80	7.80	0.15	0.15	0.15
0.81	8.04	8.04	8.04	0.17	0.17	0.17
0.91	8.27	8.27	8.27	0.22	0.22	0.22
1.02	8.49	8.49	8.49	0.27	0.27	0.27
1.13	8.70	8.70	8.70	0.33	0.33	0.33
1.23	8.86	8.86	8.86	0.39	0.39	0.39
1.34	9.05	9.05	9.05	0.45	0.45	0.45

% 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	-0.0203	-0.0203	-0.0203
0.0400	-0.0200	-0.0200	-0.0200	-0.0332	-0.0332	-0.0332
0.1500	-0.1012	-0.1012	-0.1012	-0.0861	-0.0861	-0.0861
0.2900	-0.1927	-0.1927	-0.1927	-0.1688	-0.1688	-0.1688
0.4000	-0.2567	-0.2567	-0.2567	-0.2412	-0.2412	-0.2412
0.5050	-0.3248	-0.3248	-0.3248	-0.3149	-0.3149	-0.3149
0.6050	-0.3916	-0.3916	-0.3916	-0.3885	-0.3885	-0.3885
0.7100	-0.4564	-0.4564	-0.4564	-0.4689	-0.4689	-0.4689
0.8100	-0.5324	-0.5324	-0.5324	-0.5481	-0.5481	-0.5481
0.9100	-0.6139	-0.6139	-0.6139	-0.6297	-0.6297	-0.6297
1.0200	-0.7025	-0.7025	-0.7025	-0.7219	-0.7219	-0.7219
1.1300	-0.7991	-0.7991	-0.7991	-0.8165	-0.8165	-0.8165

1.2250 -0.8883 -0.8883 -0.8883 -0.8999 -0.8999 -0.8999
 1.3400 -1.0264 -1.0264 -1.0264 -1.0029 -1.0029 -1.0029

Volume

P	P _{lin}	P _{calc,2nd}	P _{3rd}	V (Å ³)
0.0000	0.0421	0.0571	-0.0099	6518.1676
0.0400	0.0694	0.0825	0.0245	6514.2481
0.1500	0.1799	0.1860	0.1608	6498.4059
0.2900	0.3045	0.3040	0.3088	6480.5578
0.4000	0.3913	0.3873	0.4086	6468.1066
0.5050	0.4837	0.4768	0.5115	6454.8652
0.6050	0.5743	0.5654	0.6090	6441.8912
0.7100	0.6618	0.6519	0.7001	6429.3371
0.8100	0.7646	0.7545	0.8028	6414.6085
0.9100	0.8745	0.8655	0.9076	6398.8622
1.0200	0.9938	0.9877	1.0154	6381.7543
1.1300	1.1236	1.1223	1.1252	6363.1543
1.2250	1.2433	1.2481	1.2195	6345.9980
1.3400	1.4281	1.4458	1.3512	6319.5161

Input

P	σP	a	b	c	α	β	γ
0	0.1	18.679927	18.679927	18.679927	90	90	90
0.04	0.1	18.676182	18.676182	18.676182	90	90	90
0.15	0.1	18.66103	18.66103	18.66103	90	90	90
0.29	0.1	18.64393	18.64393	18.64393	90	90	90
0.4	0.1	18.631982	18.631982	18.631982	90	90	90
0.505	0.1	18.619259	18.619259	18.619259	90	90	90
0.605	0.1	18.606776	18.606776	18.606776	90	90	90
0.71	0.1	18.594681	18.594681	18.594681	90	90	90
0.81	0.1	18.580471	18.580471	18.580471	90	90	90
0.91	0.1	18.565255	18.565255	18.565255	90	90	90
1.02	0.1	18.548695	18.548695	18.548695	90	90	90
1.13	0.1	18.530657	18.530657	18.530657	90	90	90
1.225	0.1	18.513988	18.513988	18.513988	90	90	90
1.34	0.1	18.488199	18.488199	18.488199	90	90	90