

# Output

Axes			Direction				Empirical parameters		
	$K(\text{TPa}^{-1})$	$\sigma K(\text{TPa}^{-1})$	a	b	c	$\epsilon_0$	$\lambda$	$P_c$	$v$
$X_1$	11.0602	0.3760	1.0000	-0.0000	-0.0000	-8.1574e-04	-1.2697e-02	0.3300	0.8774
$X_2$	11.0602	0.3760	0.0000	1.0000	-0.0000	-8.1574e-04	-1.2697e-02	0.3300	0.8774
$X_3$	11.0608	0.3760	0.0000	0.0000	1.0000	-8.1660e-04	-1.2696e-02	0.3300	0.8775
V	34.8648	1.2348							

## Birch-Murnaghan Coefficients

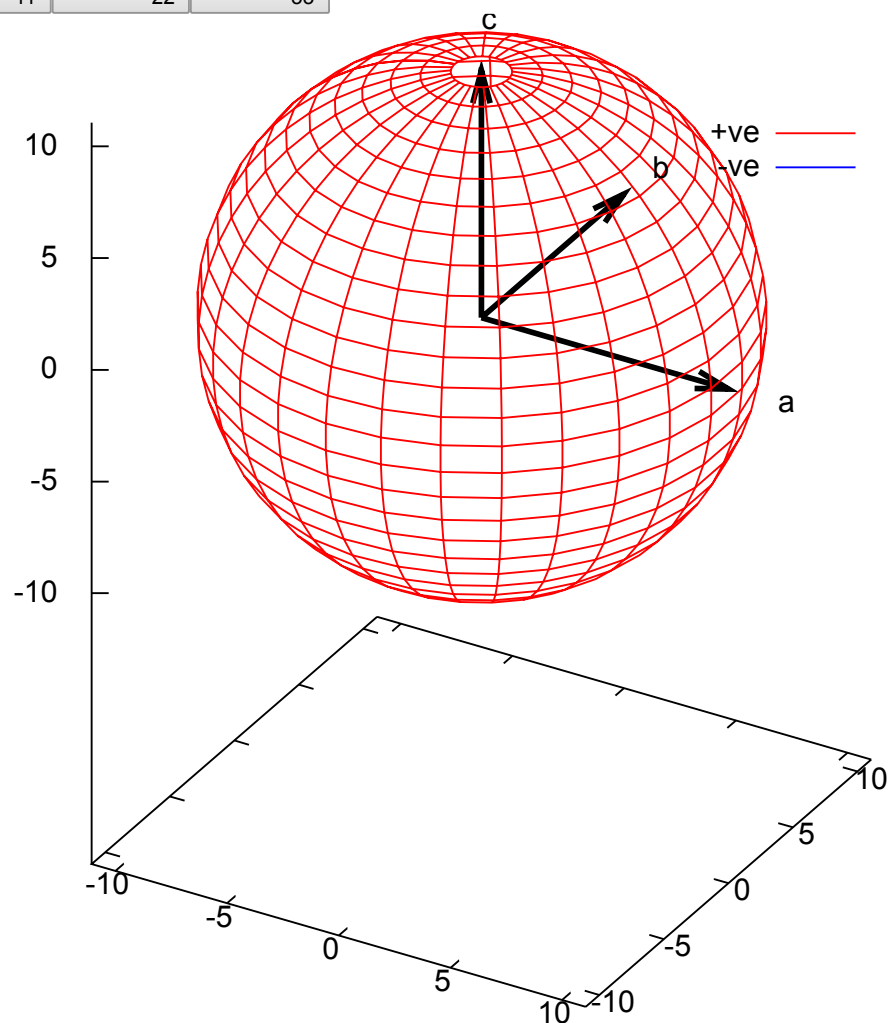
	$B_0$ (GPa)	$\sigma B_0$ (GPa)	$V_0$ ( $\text{\AA}^3$ )	$\sigma V_0$ ( $\text{\AA}^3$ )	$B'$	$\sigma B'$	$P_c$ (GPa)
2 <sup>nd</sup>	23.2146	0.5269	3149.0642	3.4888	4	n/a	0
3 <sup>rd</sup>	19.6594	2.5416	3158.3710	8.2234	7.4534	2.6674	0

## Compressibility Indicatrix

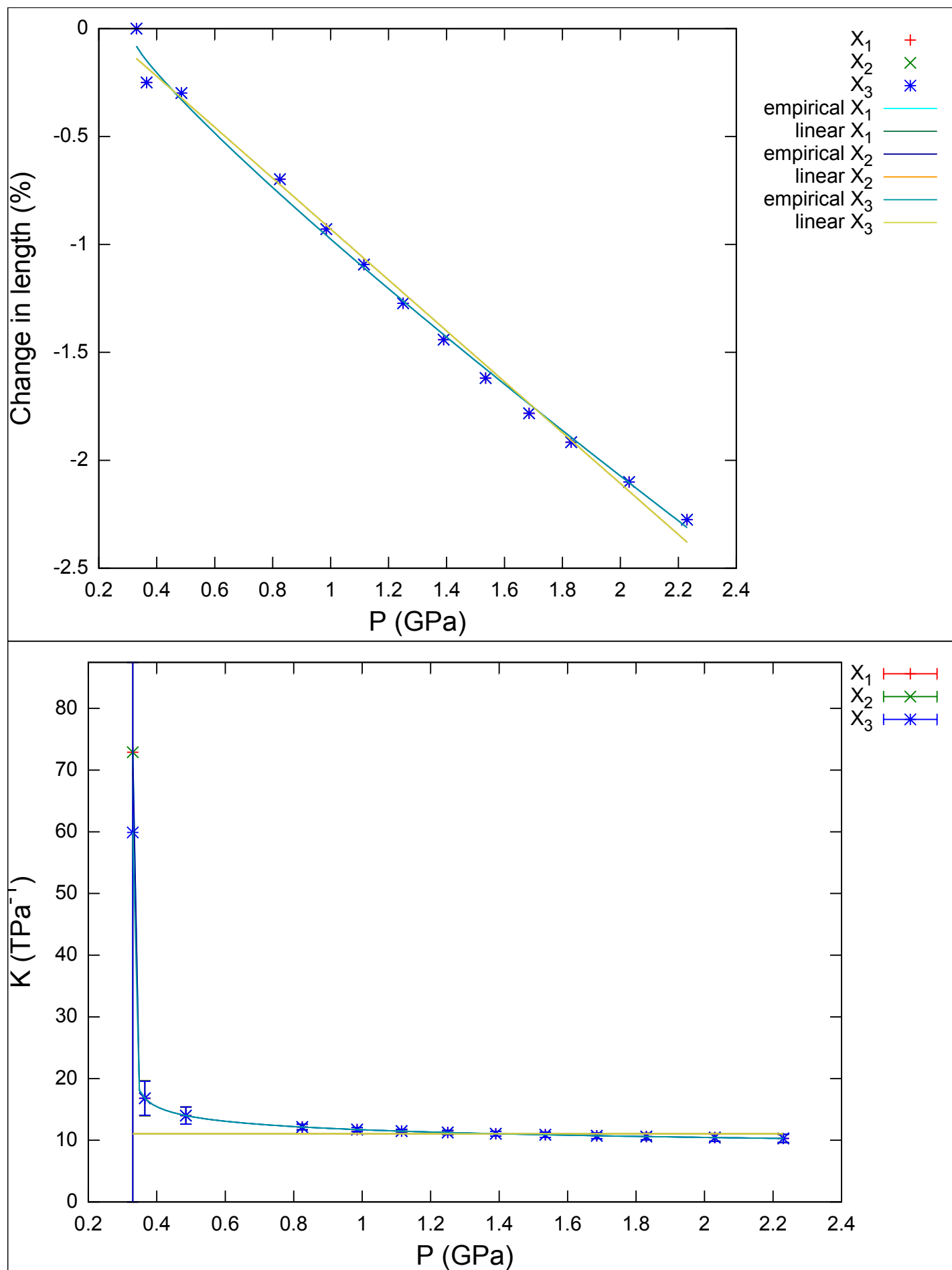
The compressibility indicatrix has units of  $\text{TPa}^{-1}$ .

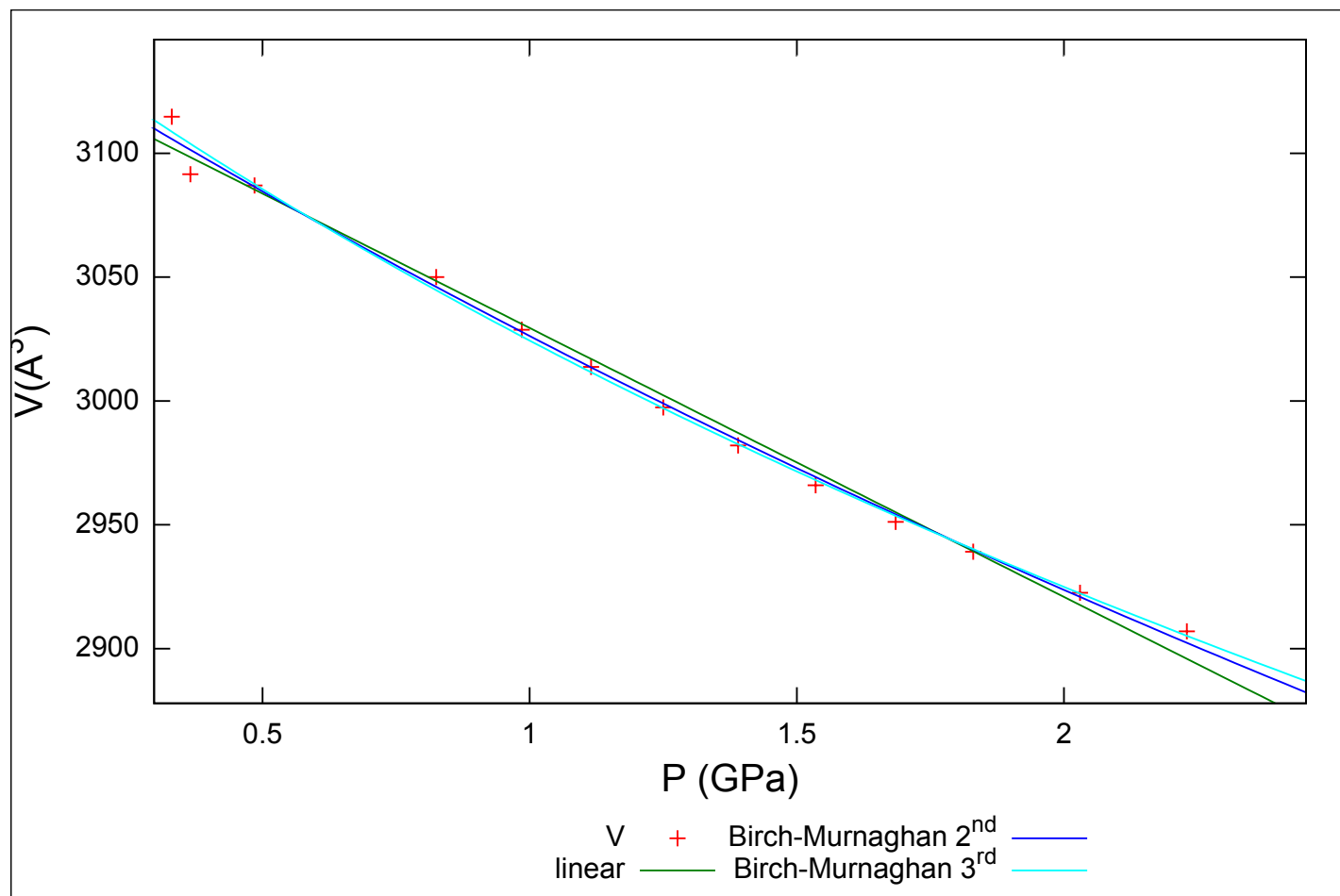
Rotate +x	Rotate -x	Rotate +z	Rotate -z
Down $e_{11}$	Down $e_{22}$	Down $e_{33}$	Value X:30

Value Z:60



## Plots





### Compressibilities (TPa<sup>-1</sup>)

P	K <sub>1</sub>	K <sub>2</sub>	K <sub>3</sub>	σK <sub>1</sub>	σK <sub>2</sub>	σK <sub>3</sub>
0.33	72.89	72.89	59.89	612890.04	612890.04	133657.47
0.36	16.80	16.80	16.80	2.84	2.84	2.75
0.48	14.00	14.00	14.00	1.39	1.39	1.38
0.82	12.14	12.14	12.14	0.45	0.45	0.45
0.98	11.73	11.73	11.73	0.32	0.32	0.32
1.11	11.48	11.48	11.48	0.30	0.30	0.30
1.25	11.25	11.25	11.25	0.33	0.33	0.33
1.39	11.06	11.06	11.06	0.38	0.38	0.38
1.53	10.89	10.89	10.89	0.43	0.43	0.43
1.69	10.73	10.73	10.73	0.49	0.49	0.49
1.83	10.60	10.60	10.60	0.54	0.54	0.54
2.03	10.44	10.44	10.44	0.61	0.61	0.61
2.23	10.30	10.30	10.30	0.66	0.66	0.67

### % change in length

P	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>1,calc</sub>	X <sub>2,calc</sub>	X <sub>3,calc</sub>
0.3300	0.0000	0.0000	0.0000	-0.0816	-0.0816	-0.0817
0.3650	-0.2493	-0.2493	-0.2493	-0.1486	-0.1486	-0.1487
0.4850	-0.2983	-0.2983	-0.2983	-0.3289	-0.3289	-0.3290
0.8250	-0.6975	-0.6975	-0.6975	-0.7667	-0.7667	-0.7667
0.9850	-0.9290	-0.9290	-0.9290	-0.9575	-0.9575	-0.9575
1.1150	-1.0928	-1.0928	-1.0928	-1.1083	-1.1083	-1.1083

1.2500 -1.2726 -1.2726 -1.2726 -1.2617 -1.2617 -1.2617  
 1.3900 -1.4413 -1.4413 -1.4413 -1.4178 -1.4178 -1.4178  
 1.5350 -1.6190 -1.6190 -1.6190 -1.5769 -1.5769 -1.5769  
 1.6850 -1.7826 -1.7826 -1.7826 -1.7390 -1.7390 -1.7391  
 1.8300 -1.9164 -1.9164 -1.9164 -1.8937 -1.8937 -1.8937  
 2.0300 -2.1009 -2.1009 -2.1009 -2.1040 -2.1040 -2.1041  
 2.2300 -2.2753 -2.2753 -2.2753 -2.3113 -2.3113 -2.3114

## Volume

P	P <sub>lin</sub>	P <sub>calc,2nd</sub>	P <sub>3rd</sub>	V (Å <sup>3</sup> )
0.3300	0.2142	0.2597	0.2876	3114.7912
0.3650	0.4282	0.4439	0.4551	3091.5538
0.4850	0.4701	0.4808	0.4890	3087.0033
0.8250	0.8102	0.7905	0.7804	3050.0659
0.9850	1.0062	0.9773	0.9614	3028.7832
1.1150	1.1443	1.1129	1.0949	3013.7847
1.2500	1.2954	1.2650	1.2470	2997.3813
1.3900	1.4366	1.4109	1.3951	2982.0417
1.5350	1.5849	1.5679	1.5568	2965.9451
1.6850	1.7209	1.7157	1.7112	2951.1680
1.8300	1.8318	1.8388	1.8412	2939.1280
2.0300	1.9843	2.0120	2.0267	2922.5700
2.2300	2.1279	2.1794	2.2085	2906.9773

## Input

P	σP	a	b	c	α	β	γ
0.33	0.1	14.604151	14.604151	14.604151	90	90	90
0.365	0.1	14.567743	14.567743	14.567743	90	90	90
0.485	0.1	14.560592	14.560592	14.560592	90	90	90
0.825	0.1	14.502284	14.502284	14.502284	90	90	90
0.985	0.1	14.468474	14.468474	14.468474	90	90	90
1.115	0.1	14.444552	14.444552	14.444552	90	90	90
1.25	0.1	14.418298	14.418298	14.418298	90	90	90
1.39	0.1	14.39366	14.39366	14.39366	90	90	90
1.535	0.1	14.367715	14.367715	14.367715	90	90	90
1.685	0.1	14.343814	14.343814	14.343814	90	90	90
1.83	0.1	14.324281	14.324281	14.324281	90	90	90
2.03	0.1	14.297331	14.297331	14.297331	90	90	90
2.23	0.1	14.271859	14.271859	14.271859	90	90	90