

## Output

Axes			Direction				Empirical parameters		
	$K(\text{TPa}^{-1})$	$\sigma K(\text{TPa}^{-1})$	a	b	c	$\epsilon_0$	$\lambda$	$P_c$	$v$
$X_1$	8.6162	0.7606	0.7071	-0.7071	0.0000	-3.4749e-05	-8.5658e-03	0.1600	1.0149
$X_2$	8.6162	0.7606	0.0000	0.0000	1.0000	-3.4749e-05	-8.5658e-03	0.1600	1.0149
$X_3$	8.6163	0.7613	-0.7071	-0.7071	0.0000	-3.4880e-05	-8.5658e-03	0.1600	1.0149
$V$	25.3438	0.7221							

## Birch-Murnaghan Coefficients

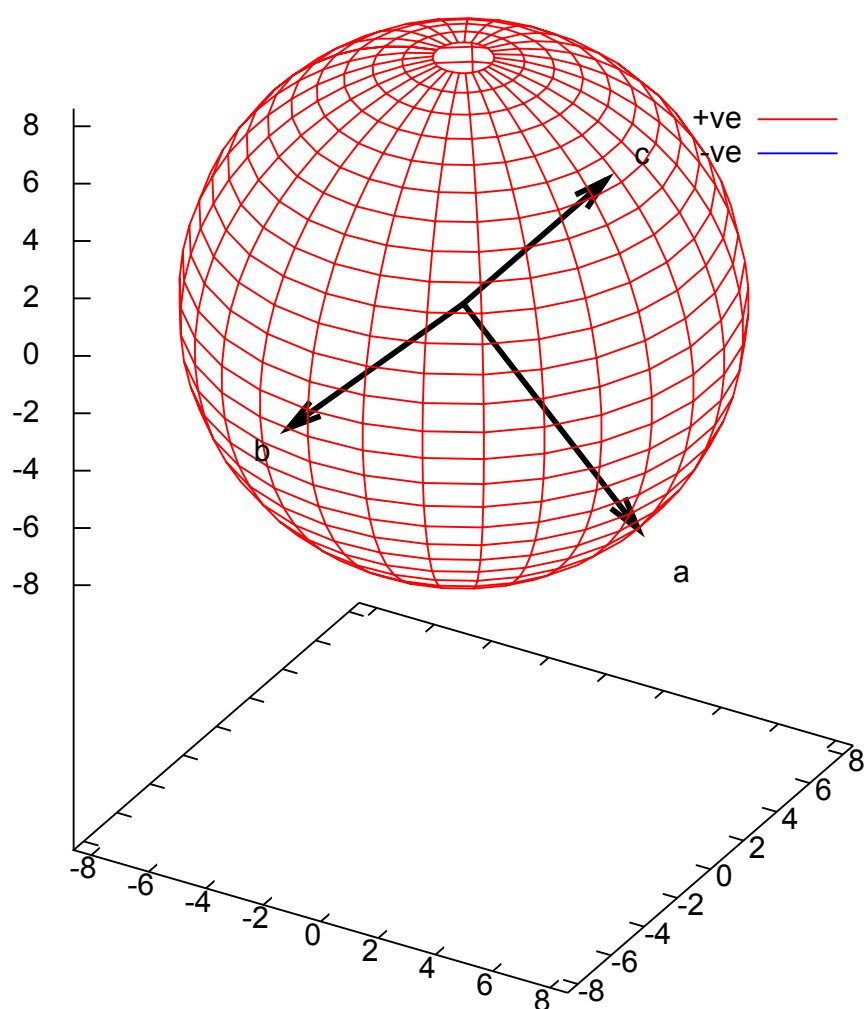
	$B_0$ (GPa)	$\sigma B_0$ (GPa)	$V_0$ ( $\text{\AA}^3$ )	$\sigma V_0$ ( $\text{\AA}^3$ )	$B'$	$\sigma B'$	$P_c$ (GPa)
2 <sup>nd</sup>	36.8402	1.5600	3386.1236	2.2389	4	n/a	0
3 <sup>rd</sup>	38.5145	9.0519	3385.2563	5.0450	1.0507	15.2789	0

## Compressibility Indicatrix

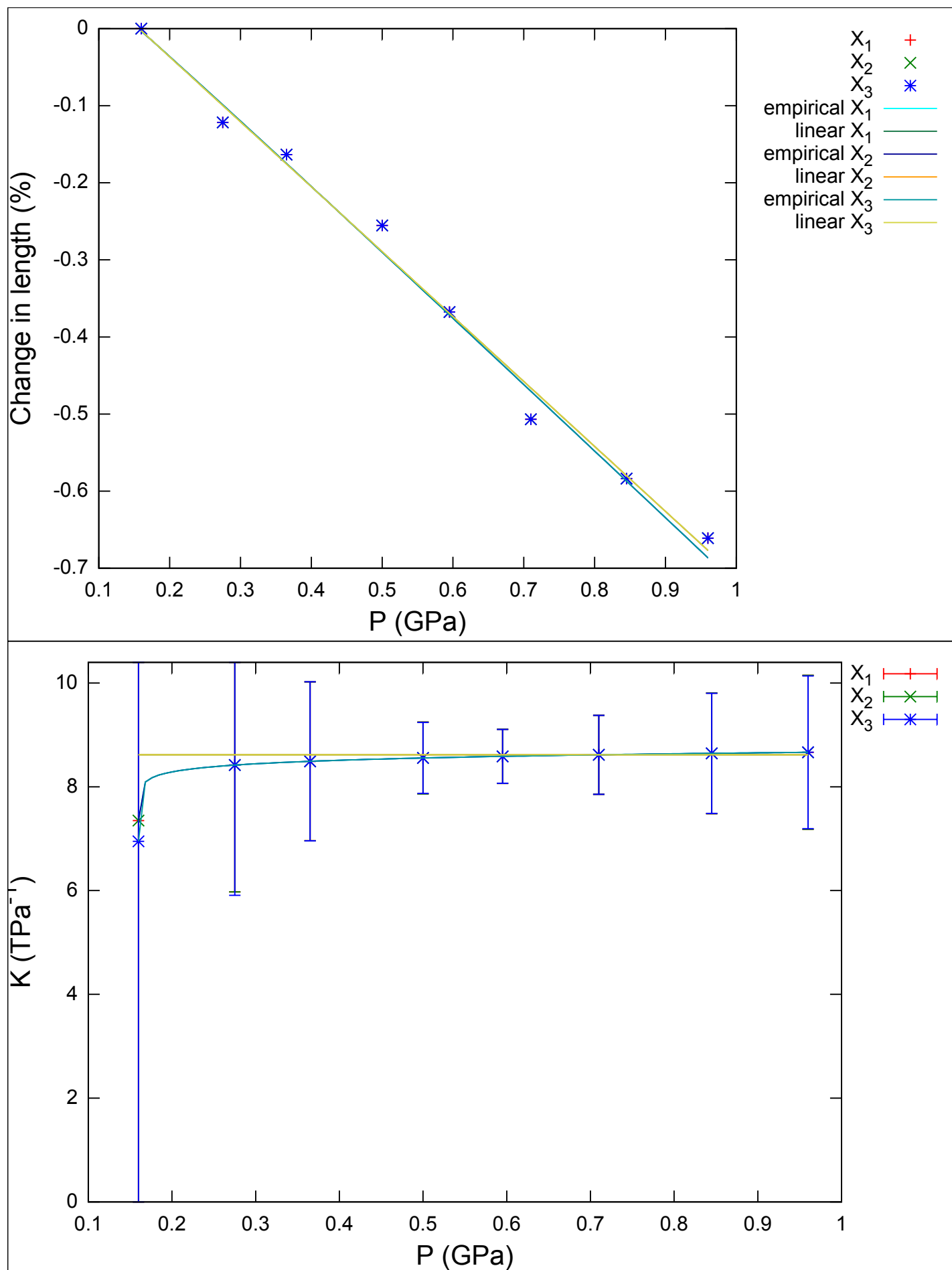
The compressibility indicatrix has units of  $\text{TPa}^{-1}$ .

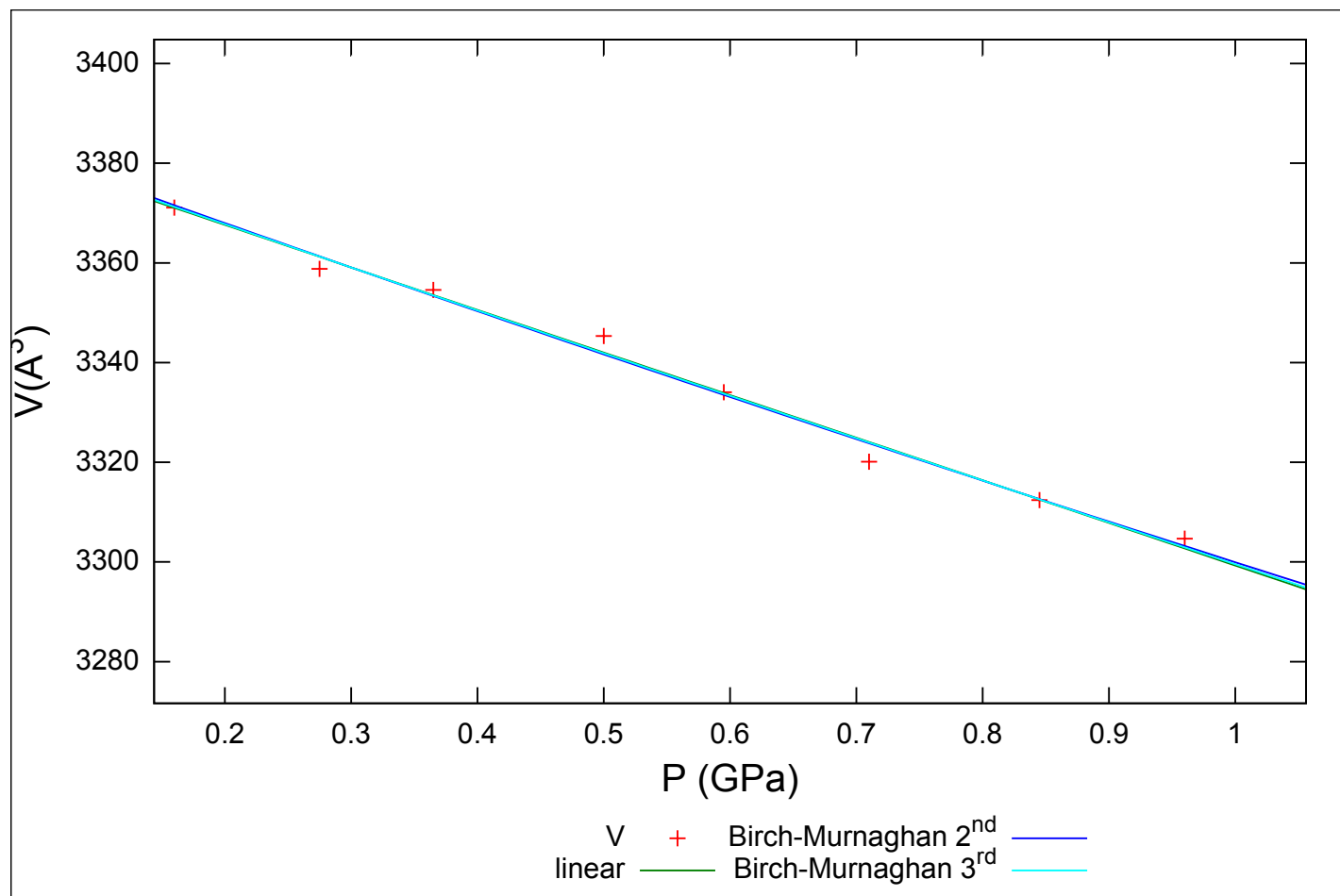
Rotate +x	Rotate -x	Rotate +z	Rotate -z
Down $e_{11}$	Down $e_{22}$	Down $e_{33}$	Value X:30

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>
0.16	7.35	7.35	6.95	7475.66	7475.66	214008.68
0.28	8.42	8.42	8.42	2.44	2.44	2.51
0.36	8.49	8.49	8.49	1.53	1.53	1.53
0.50	8.55	8.55	8.55	0.69	0.69	0.68
0.59	8.59	8.59	8.59	0.52	0.52	0.52
0.71	8.62	8.62	8.62	0.76	0.76	0.76
0.84	8.64	8.64	8.64	1.16	1.16	1.16
0.96	8.66	8.66	8.66	1.48	1.48	1.47

### % 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>
0.1600	0.0000	0.0000	0.0000	-0.0035	-0.0035	-0.0035
0.2750	-0.1218	-0.1218	-0.1218	-0.0989	-0.0989	-0.0989
0.3650	-0.1634	-0.1634	-0.1634	-0.1750	-0.1750	-0.1750
0.5000	-0.2554	-0.2554	-0.2554	-0.2901	-0.2901	-0.2901
0.5950	-0.3677	-0.3677	-0.3677	-0.3715	-0.3715	-0.3715
0.7100	-0.5068	-0.5068	-0.5068	-0.4704	-0.4704	-0.4704
0.8450	-0.5837	-0.5837	-0.5837	-0.5869	-0.5869	-0.5869
0.9600	-0.6610	-0.6610	-0.6610	-0.6865	-0.6865	-0.6865

### Volume

<b>P</b>	<b>P<sub>lin</sub></b>	<b>P<sub>calc,2nd</sub></b>	<b>P<sub>3rd</sub></b>	<b>V (Å<sup>3</sup>)</b>
0.1600	0.1596	0.1654	0.1618	3371.0933
0.2750	0.3035	0.3034	0.3035	3358.7943
0.3650	0.3527	0.3512	0.3521	3354.5921
0.5000	0.4611	0.4575	0.4597	3345.3293
0.5950	0.5933	0.5890	0.5917	3334.0398
0.7100	0.7564	0.7545	0.7557	3320.1029
0.8450	0.8465	0.8474	0.8468	3312.4087
0.9600	0.9369	0.9416	0.9387	3304.6832

## Input

<b>P</b>	<b>σP</b>	<b>a</b>	<b>b</b>	<b>c</b>	<b>α</b>	<b>β</b>	<b>γ</b>
0.16	0.1	14.99421	14.99421	14.99421	90	90	90
0.275	0.1	14.975953	14.975953	14.975953	90	90	90
0.365	0.1	14.969705	14.969705	14.969705	90	90	90
0.5	0.1	14.955914	14.955914	14.955914	90	90	90
0.595	0.1	14.939071	14.939071	14.939071	90	90	90
0.71	0.1	14.918226	14.918226	14.918226	90	90	90
0.845	0.1	14.906693	14.906693	14.906693	90	90	90
0.96	0.1	14.895095	14.895095	14.895095	90	90	90