

# Output

Axes	Direction			Empirical parameters					$P_c$	$v$
	$K(\text{TPa}^{-1})$	$\sigma K(\text{TPa}^{-1})$	a	b	c	$\epsilon_0$	$\lambda$			
$X_1$	10.3916	0.2386	1.0000	-0.0000	-0.0000	-3.5524e-04	-7.9383e-03		0.0000	1.4460
$X_2$	10.3916	0.2386	0.0000	1.0000	-0.0000	-3.5524e-04	-7.9383e-03		0.0000	1.4460
$X_3$	10.3916	0.2386	0.0000	0.0000	1.0000	-3.5524e-04	-7.9383e-03		0.0000	1.4460
V	27.6156	1.3997								

## Birch-Murnaghan Coefficients

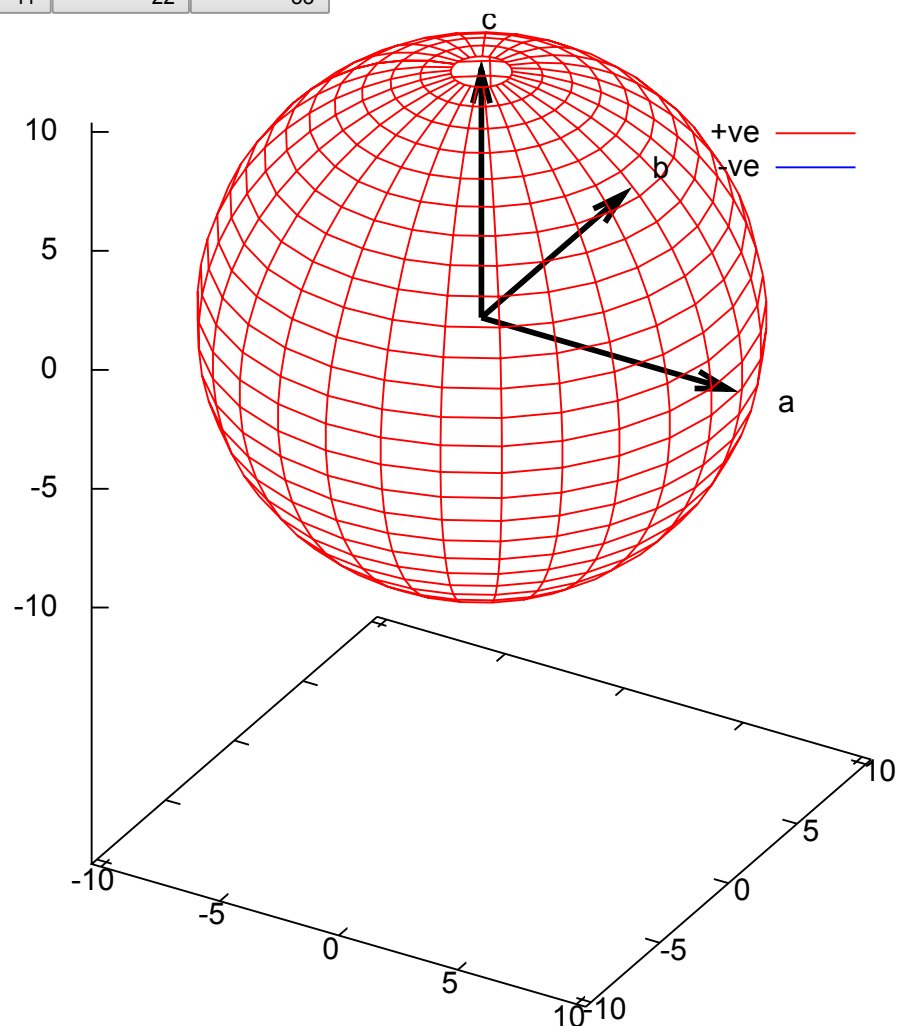
	$B_0$ (GPa)	$\sigma B_0$ (GPa)	$V_0$ ( $\text{\AA}^3$ )	$\sigma V_0$ ( $\text{\AA}^3$ )	$B'$	$\sigma B'$	$P_c$ (GPa)
2 <sup>nd</sup>	32.4510	1.6994	6551.1291	7.5421	4	n/a	0
3 <sup>rd</sup>	52.5963	0.6112	6528.1980	0.6658	-16.1547	0.4518	0

## Compressibility Indicatrix

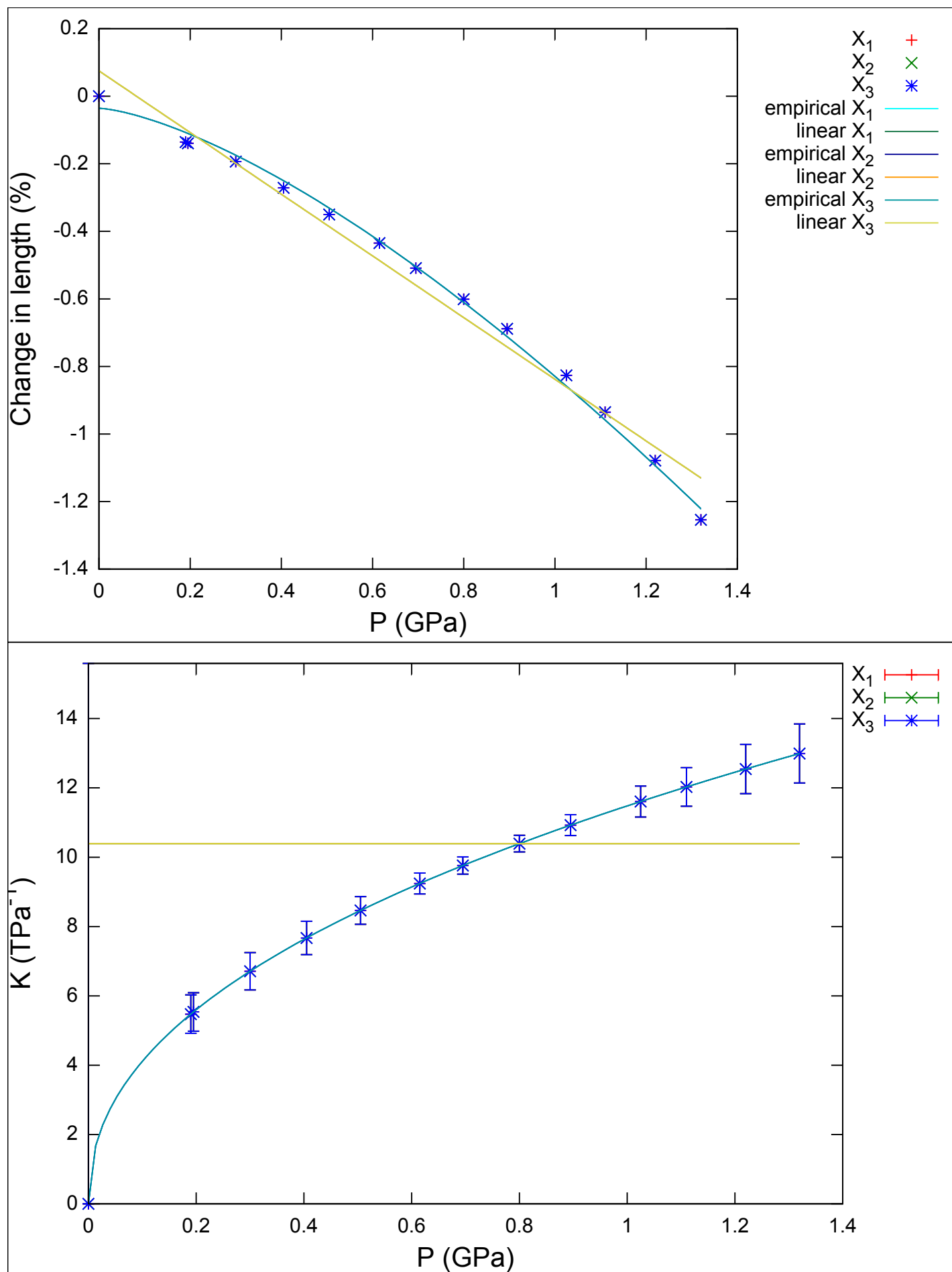
The compressibility indicatrix has units of  $\text{TPa}^{-1}$ .

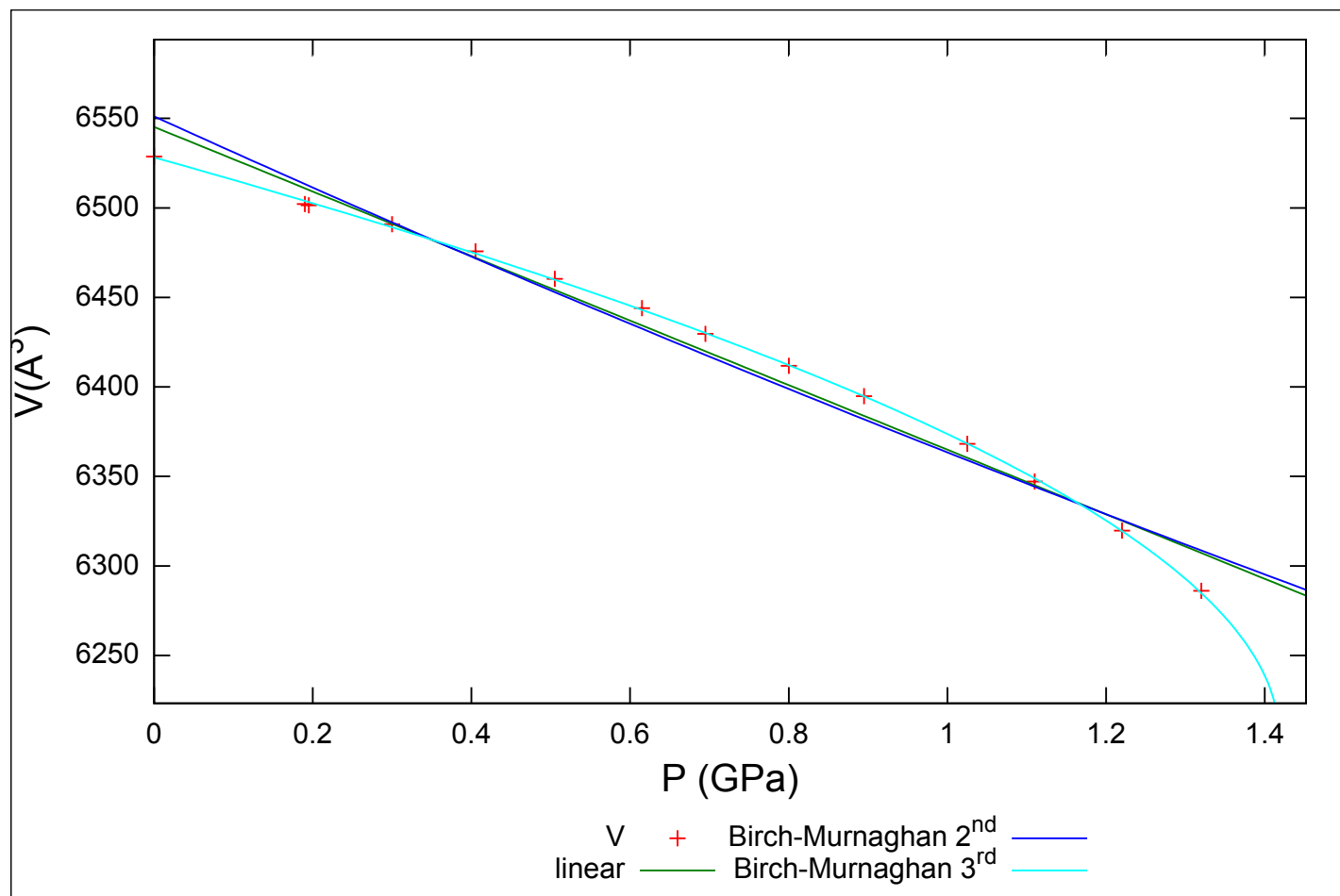
Rotate +x	Rotate -x	Rotate +z	Rotate -z
Down e <sub>11</sub>	Down e <sub>22</sub>	Down e <sub>33</sub>	Value X:30

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>
0.00	0.00	0.00	0.00	304607006927966016.00	304607006927966016.00	304607006927966016.00
0.19	5.47	5.47	5.47	0.55	0.55	0.55
0.20	5.54	5.54	5.54	0.55	0.55	0.55
0.30	6.71	6.71	6.71	0.54	0.54	0.54
0.41	7.67	7.67	7.67	0.48	0.48	0.48
0.51	8.46	8.46	8.46	0.40	0.40	0.40
0.61	9.24	9.24	9.24	0.30	0.30	0.30
0.69	9.76	9.76	9.76	0.25	0.25	0.25
0.80	10.39	10.39	10.39	0.24	0.24	0.24
0.90	10.92	10.92	10.92	0.30	0.30	0.30
1.02	11.61	11.61	11.61	0.45	0.45	0.45
1.11	12.03	12.03	12.03	0.56	0.56	0.56
1.22	12.54	12.54	12.54	0.71	0.71	0.71
1.32	12.99	12.99	12.99	0.85	0.85	0.85

### % 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>
0.0000	0.0000	0.0000	0.0000	-0.0355	-0.0355	-0.0355
0.1900	-0.1357	-0.1357	-0.1357	-0.1074	-0.1074	-0.1074
0.1950	-0.1395	-0.1395	-0.1395	-0.1102	-0.1102	-0.1102
0.3000	-0.1934	-0.1934	-0.1934	-0.1747	-0.1747	-0.1747
0.4050	-0.2713	-0.2713	-0.2713	-0.2504	-0.2504	-0.2504

0.5050 -0.3504 -0.3504 -0.3504 -0.3311 -0.3311 -0.3311  
 0.6150 -0.4347 -0.4347 -0.4347 -0.4286 -0.4286 -0.4286  
 0.6950 -0.5087 -0.5087 -0.5087 -0.5046 -0.5046 -0.5046  
 0.8000 -0.6008 -0.6008 -0.6008 -0.6104 -0.6104 -0.6104  
 0.8950 -0.6884 -0.6884 -0.6884 -0.7117 -0.7117 -0.7117  
 1.0250 -0.8264 -0.8264 -0.8264 -0.8582 -0.8582 -0.8582  
 1.1100 -0.9356 -0.9356 -0.9356 -0.9587 -0.9587 -0.9587  
 1.2200 -1.0787 -1.0787 -1.0787 -1.0938 -1.0938 -1.0938  
 1.3200 -1.2543 -1.2543 -1.2543 -1.2215 -1.2215 -1.2215

## Volume

P	P <sub>lin</sub>	P <sub>calc,2nd</sub>	P <sub>3rd</sub>	V (Å <sup>3</sup> )
0.0000	0.0914	0.1119	-0.0043	6528.7326
0.1900	0.2387	0.2470	0.2032	6502.1853
0.1950	0.2427	0.2508	0.2087	6501.4506
0.3000	0.3012	0.3052	0.2871	6490.9172
0.4050	0.3853	0.3844	0.3961	6475.7403
0.5050	0.4707	0.4656	0.5018	6460.3488
0.6150	0.5616	0.5532	0.6089	6443.9698
0.6950	0.6413	0.6308	0.6980	6429.6006
0.8000	0.7402	0.7285	0.8022	6411.7587
0.8950	0.8341	0.8224	0.8944	6394.8314
1.0250	0.9818	0.9725	1.0257	6368.2106
1.1100	1.0984	1.0933	1.1170	6347.1879
1.2200	1.2507	1.2541	1.2193	6319.7222
1.3200	1.4370	1.4554	1.3169	6286.1231

## Input

P	σP	a	b	c	α	β	γ
0	0.1	18.690014	18.690014	18.690014	90	90	90
0.195	0.1	18.663944	18.663944	18.663944	90	90	90
0.19	0.1	18.664647	18.664647	18.664647	90	90	90
0.3	0.1	18.653859	18.653859	18.653859	90	90	90
0.405	0.1	18.639309	18.639309	18.639309	90	90	90
0.505	0.1	18.62453	18.62453	18.62453	90	90	90
0.615	0.1	18.608777	18.608777	18.608777	90	90	90
0.695	0.1	18.594935	18.594935	18.594935	90	90	90
0.8	0.1	18.577719	18.577719	18.577719	90	90	90
0.895	0.1	18.561356	18.561356	18.561356	90	90	90
1.025	0.1	18.535564	18.535564	18.535564	90	90	90
1.11	0.1	18.515145	18.515145	18.515145	90	90	90
1.22	0.1	18.4884	18.4884	18.4884	90	90	90
1.32	0.1	18.455577	18.455577	18.455577	90	90	90