

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	32.5967	1.3254	0.0000	0.0000	1.0000	1.6490e-04	-1.3937e-02	0.0000	1.6126
X_2	6.8944	0.2527	-0.7071	-0.7071	0.0000	-2.0099e-05	-6.6459e-03	0.0000	1.0230
X_3	6.8944	0.2527	0.7071	-0.7071	0.0000	-2.0099e-05	-6.6459e-03	0.0000	1.0230
V	33.8928	1.2067							

Birch-Murnaghan Coefficients

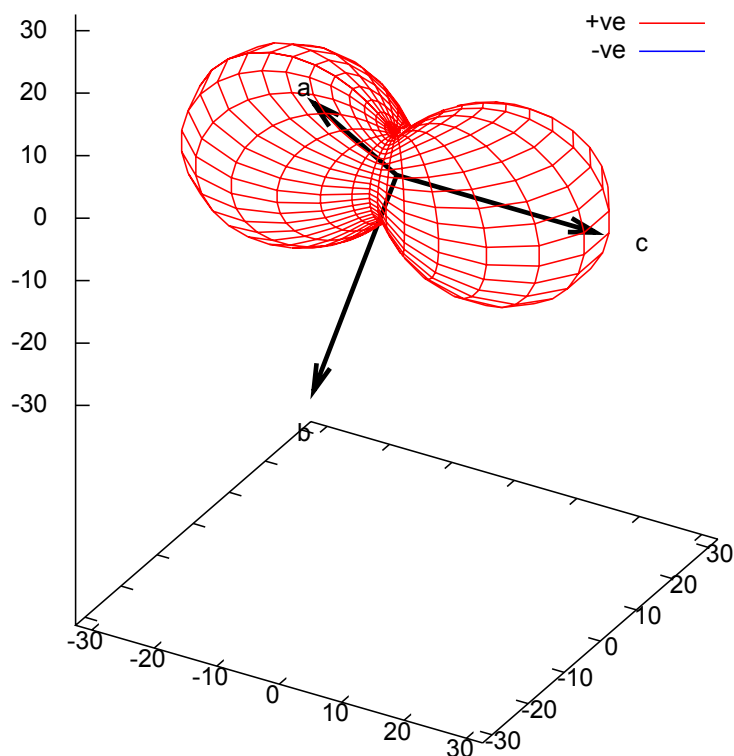
	B_0 (GPa)	σB_0 (GPa)	V_0 (\AA^3)	σV_0 (\AA^3)	B'	$\sigma B'$	P_c (GPa)
2 nd	24.2877	1.8363	6556.3104	26.7044	4	n/a	0
3 rd	37.2710	0.7327	6529.1084	2.5960	-5.5176	0.3908	0

Compressibility Indicatrix

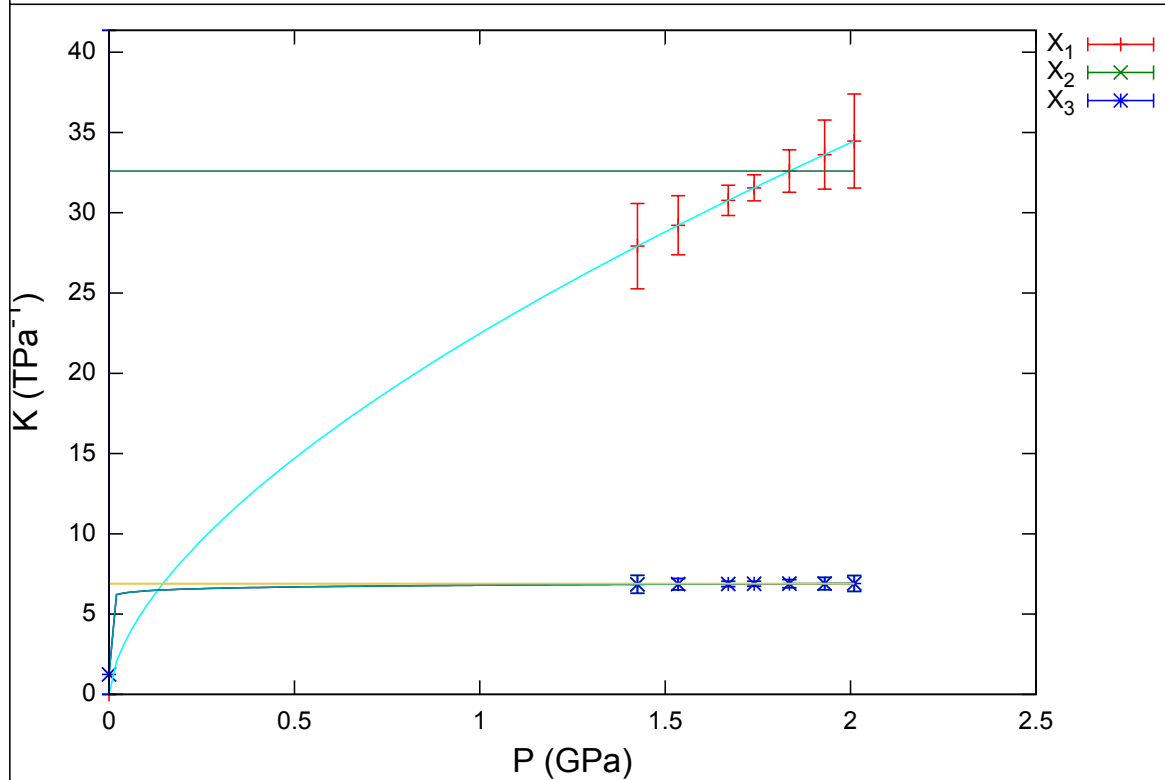
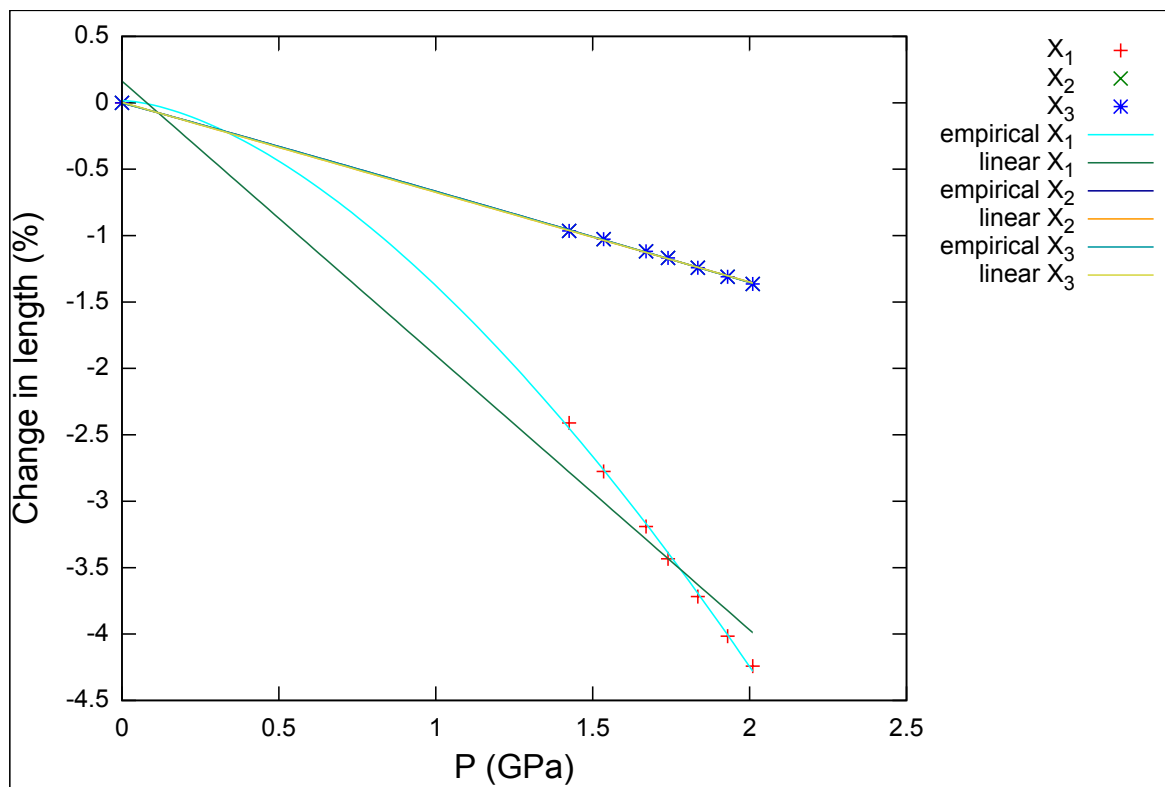
The compressibility indicatrix has units of TPa^{-1} .

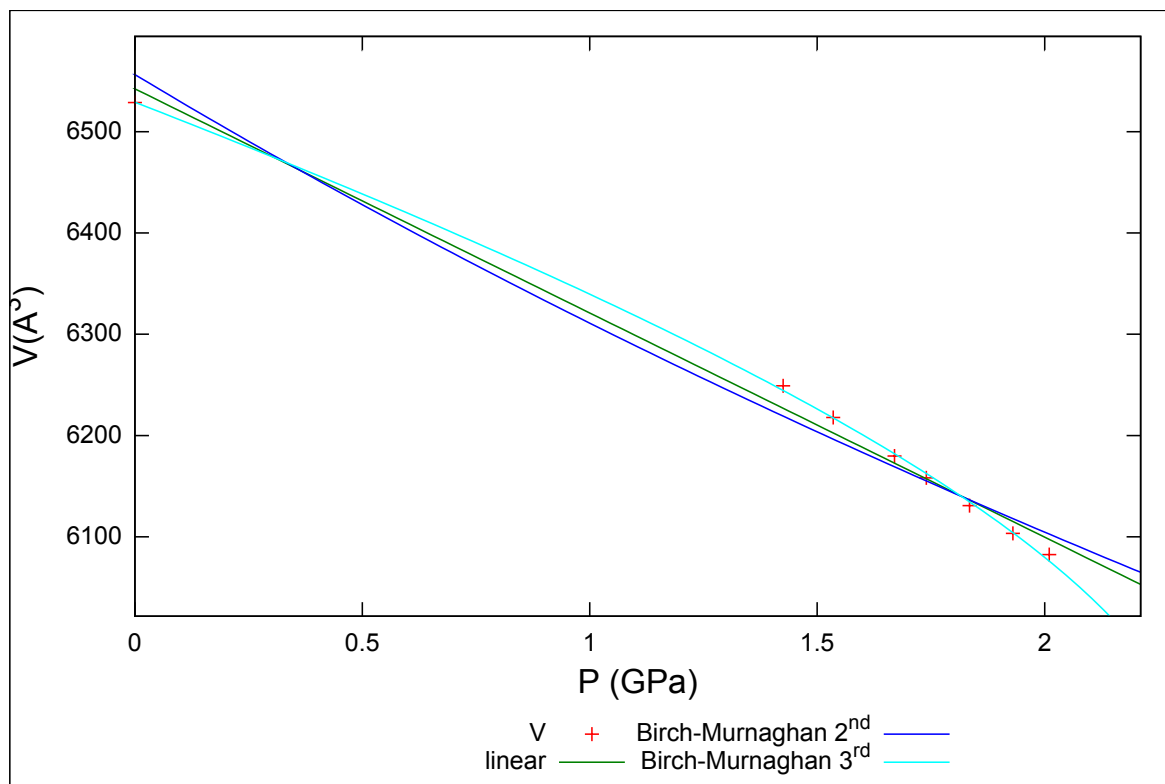
Rotate +x	Rotate -x	Rotate +z	Rotate -z
Down e_{11}	Down e_{22}	Down e_{33}	Value X:30

Value Z:60



Plots





Compressibilities (TPa⁻¹)

P	K ₁	K ₂	K ₃	σK ₁	σK ₂	σK ₃
0.00	0.00	1.24	1.24	32689302557833.59	3203830840462298699971883433984.00	3203827014845648222012844277760.00
1.43	27.92	6.85	6.85	2.66	0.56	0.56
1.53	29.22	6.87	6.87	1.84	0.35	0.35
1.67	30.77	6.88	6.88	0.94	0.17	0.17
1.74	31.55	6.89	6.89	0.81	0.16	0.16
1.83	32.60	6.89	6.89	1.33	0.25	0.25
1.93	33.62	6.90	6.90	2.15	0.38	0.38
2.01	34.47	6.91	6.91	2.93	0.50	0.50

% 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	0.0165	-0.0020	-0.0020
1.4250	-2.4100	-0.9643	-0.9643	-2.4507	-0.9568	-0.9568
1.5350	-2.7756	-1.0265	-1.0265	-2.7650	-1.0323	-1.0323
1.6700	-3.1909	-1.1182	-1.1182	-3.1700	-1.1250	-1.1250
1.7400	-3.4333	-1.1675	-1.1675	-3.3881	-1.1732	-1.1732
1.8350	-3.7176	-1.2416	-1.2416	-3.6928	-1.2387	-1.2387
1.9300	-4.0163	-1.3100	-1.3100	-4.0074	-1.3042	-1.3042
2.0100	-4.2414	-1.3637	-1.3637	-4.2797	-1.3595	-1.3595

Volume

P	P _{lin}	P _{calc,2nd}	P _{3rd}	V (Å ³)
0.0000	0.0611	0.1032	0.0021	6528.7326
1.4250	1.3248	1.2831	1.4059	6249.0999
1.5350	1.4659	1.4313	1.5331	6217.8733
1.6700	1.6377	1.6166	1.6778	6179.8523
1.7400	1.7355	1.7245	1.7549	6158.2306
1.8350	1.8590	1.8635	1.8466	6130.8977
1.9300	1.9832	2.0063	1.9321	6103.4174
2.0100	2.0778	2.1171	1.9925	6082.4735

Input

P	σP	a	b	c	α	β	γ
0	0.1	18.690014	18.690014	18.690014	90	90	90
1.425	0.1	18.509783	18.509783	18.239579	90	90	90
1.535	0.1	18.498155	18.498155	18.17126	90	90	90
1.67	0.1	18.481029	18.481029	18.093634	90	90	90
1.74	0.1	18.471812	18.471812	18.048327	90	90	90
1.835	0.1	18.457967	18.457967	17.995186	90	90	90
1.93	0.1	18.445184	18.445184	17.939366	90	90	90
2.01	0.1	18.435141	18.435141	17.897291	90	90	90