

Output

Axes			Direction			Empirical parameters			P_c	ν
	$K(\text{TPa}^{-1})$	$\sigma K(\text{TPa}^{-1})$	a	b	c	ϵ_0	λ			
X_1	32.7740	4.9419	0.0000	0.0000	1.0000	6.2469e-04	-1.9638e-02		0.0000	1.3282
X_2	8.0052	0.2466	-0.9732	-0.2298	0.0000	2.3326e-05	-6.7367e-03		0.0000	1.1048
X_3	8.0052	0.2466	-0.2298	0.9732	-0.0000	2.3325e-05	-6.7367e-03		0.0000	1.1048
V	38.7797	1.0545								

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	20.2091	1.5298	6552.9494	33.0223	4	n/a	0
3 rd	30.5955	1.6583	6519.4954	8.7691	-3.2234	0.8480	0

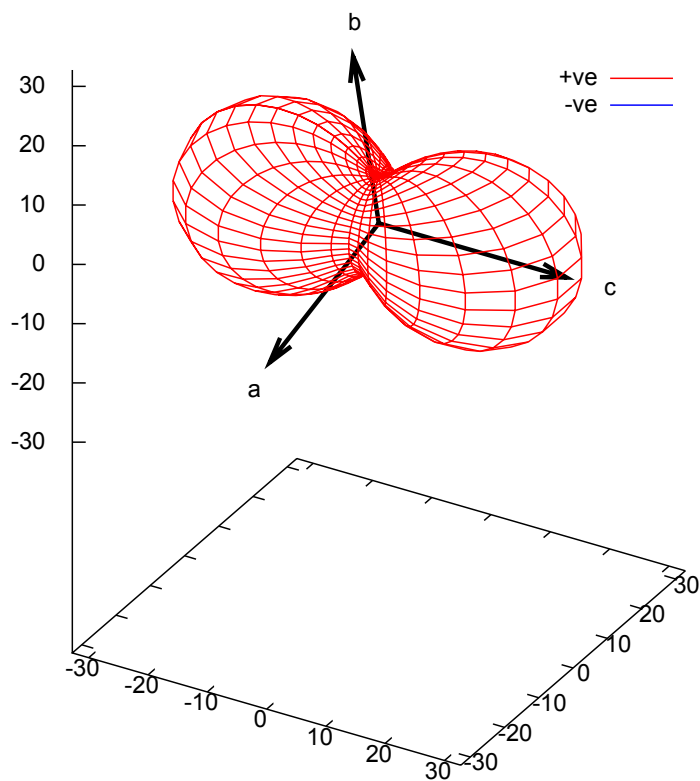
Compressibility Indicatrix

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

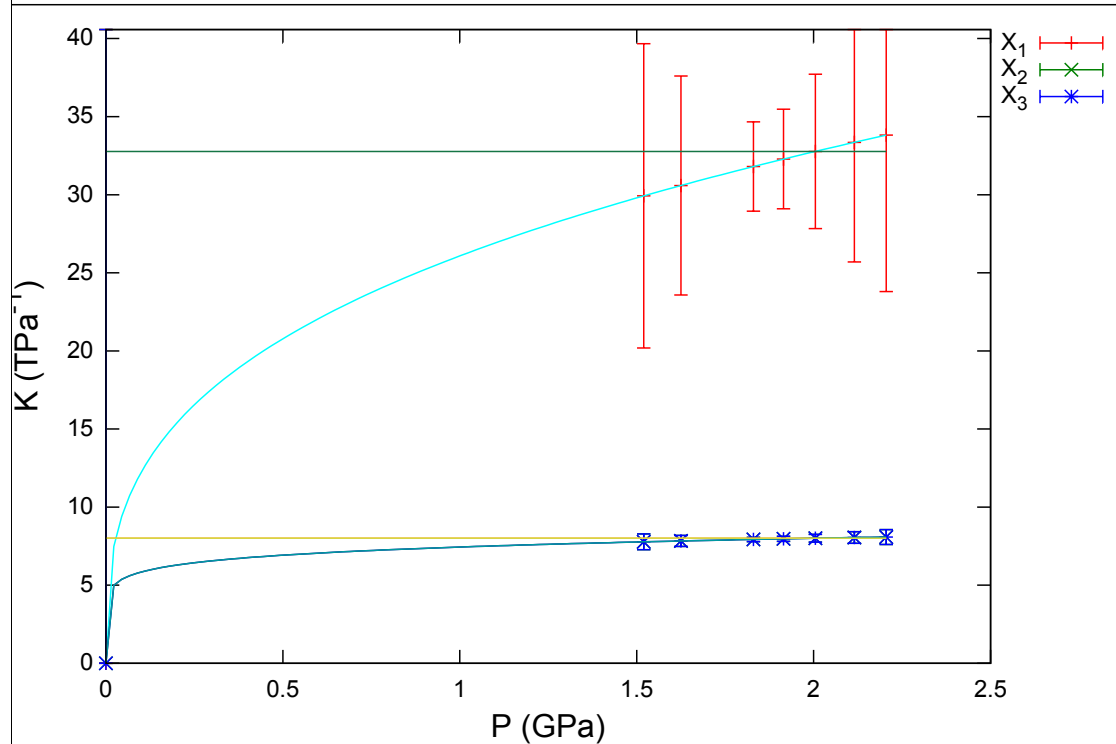
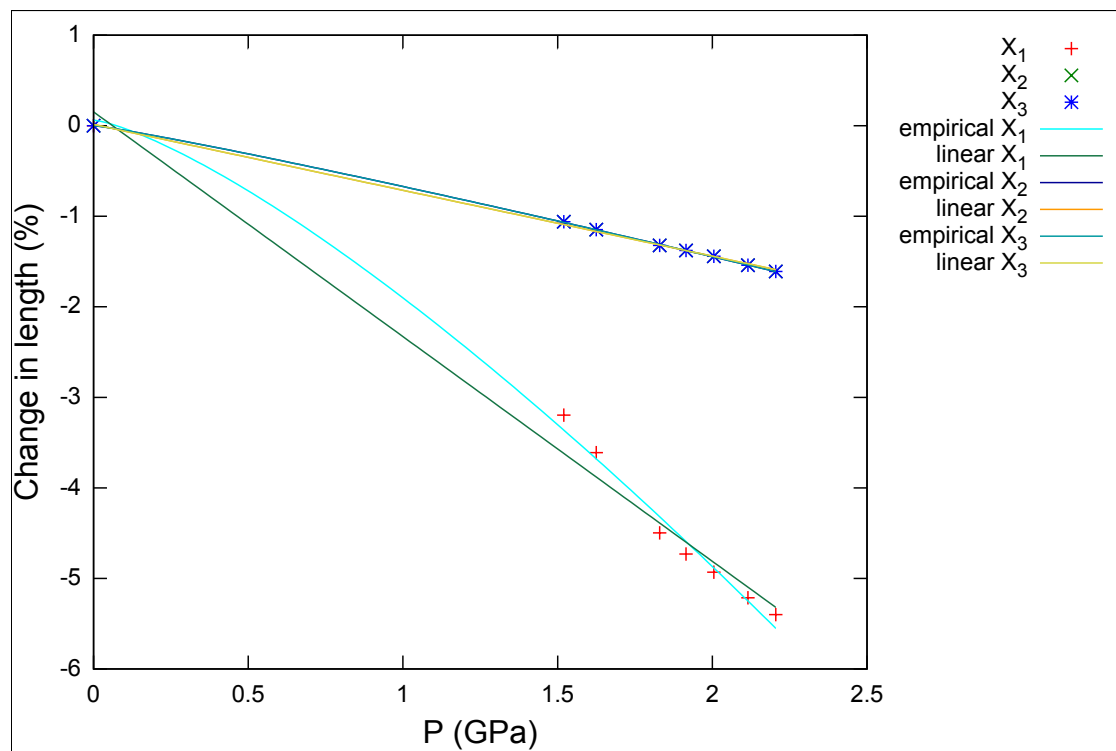
Rotate +x	Rotate -x	Rotate +z	Rotate -z
Down e_{11}	Down e_{22}	Down e_{33}	

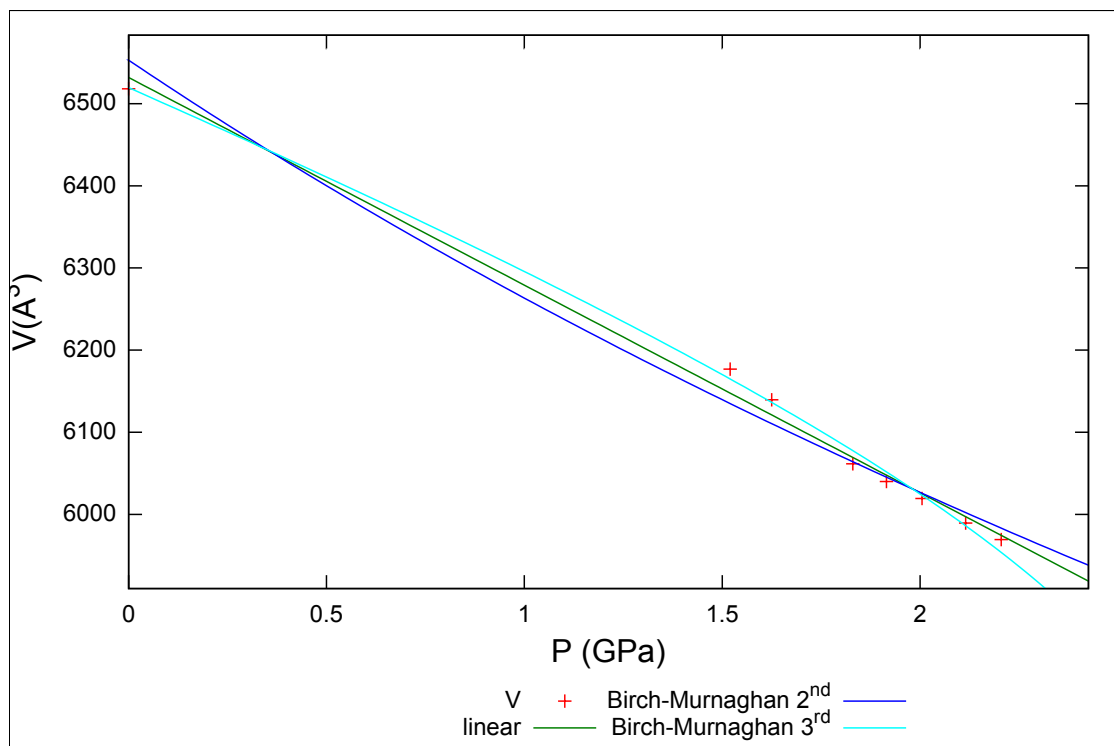
Value X:30

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	92871534929050788167680.00	25000654398544613674456186880.00	25000571757213556459003969536.00
1.52	29.93	7.78	7.78	9.74	0.51	0.51
1.62	30.59	7.83	7.83	7.01	0.35	0.35
1.83	31.81	7.93	7.93	2.86	0.14	0.14
1.92	32.28	7.97	7.97	3.19	0.16	0.16
2.00	32.77	8.01	8.01	4.94	0.25	0.25
2.12	33.35	8.05	8.05	7.66	0.37	0.37
2.21	33.81	8.09	8.09	10.01	0.48	0.48

% 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	0.0625	0.0023	0.0023
1.5200	-3.1959	-1.0598	-1.0598	-3.3623	-1.0676	-1.0676
1.6250	-3.6103	-1.1474	-1.1474	-3.6800	-1.1495	-1.1495
1.8300	-4.4963	-1.3216	-1.3216	-4.3197	-1.3111	-1.3111
1.9150	-4.7299	-1.3770	-1.3770	-4.5921	-1.3786	-1.3786
2.0050	-4.9305	-1.4416	-1.4416	-4.8849	-1.4505	-1.4505
2.1150	-5.2135	-1.5413	-1.5413	-5.2486	-1.5388	-1.5388
2.2050	-5.3994	-1.6091	-1.6091	-5.5509	-1.6114	-1.6114

Volume

P	P _{lin}	P _{calc,2nd}	P _{3rd}	V (Å ³)
0.0000	0.0541	0.1087	0.0062	6518.1676
1.5200	1.4045	1.3446	1.4750	6176.8190
1.6250	1.5522	1.5006	1.6135	6139.4869
1.8300	1.8602	1.8409	1.8828	6061.6331
1.9150	1.9457	1.9391	1.9525	6040.0239
2.0050	2.0272	2.0343	2.0166	6019.4134
2.1150	2.1461	2.1759	2.1059	5989.3570
2.2050	2.2251	2.2719	2.1625	5969.3794

Input

P σP a b c α β γ

0	0.1	18.679927	18.679927	18.679927	90	90	90
1.52	0.1	18.481961	18.481961	18.082929	90	90	90
1.625	0.1	18.465585	18.465585	18.005531	90	90	90
1.83	0.1	18.433047	18.433047	17.840022	90	90	90
1.915	0.1	18.422706	18.422706	17.796386	90	90	90
2.005	0.1	18.410645	18.410645	17.758904	90	90	90
2.115	0.1	18.39201	18.39201	17.706055	90	90	90
2.205	0.1	18.379342	18.379342	17.671331	90	90	90