

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	8.9019	0.1171	0.0000	0.0000	1.0000	-1.8441e-04	-7.5380e-03	0.0000	1.1820
X_2	7.2526	0.0933	-0.3622	-0.9321	0.0000	-9.5290e-05	-6.3315e-03	0.0000	1.1463
X_3	7.2526	0.0933	-0.9906	-0.1369	0.0000	-9.5290e-05	-6.3315e-03	0.0000	1.1463
V	22.4395	0.4587							

Birch-Murnaghan Coefficients

	B_0 (GPa)	σB_0 (GPa)	V_0 (Å ³)	σV_0 (Å ³)	B'	$\sigma B'$	P_c (GPa)
2 nd	39.5873	1.1523	7401.0870	5.4156	4	n/a	0
3 rd	51.8308	1.6120	7384.1809	2.5139	-6.5406	1.1471	0

Compressibility Indicatrix

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

Rotate +x

Rotate -x

Rotate +z

Rotate -z

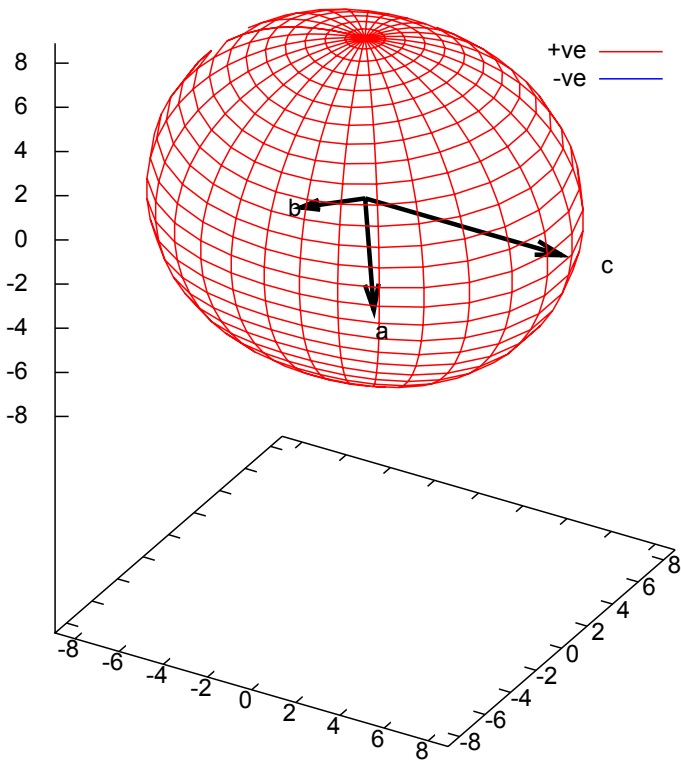
Down e_{11}

Down e_{22}

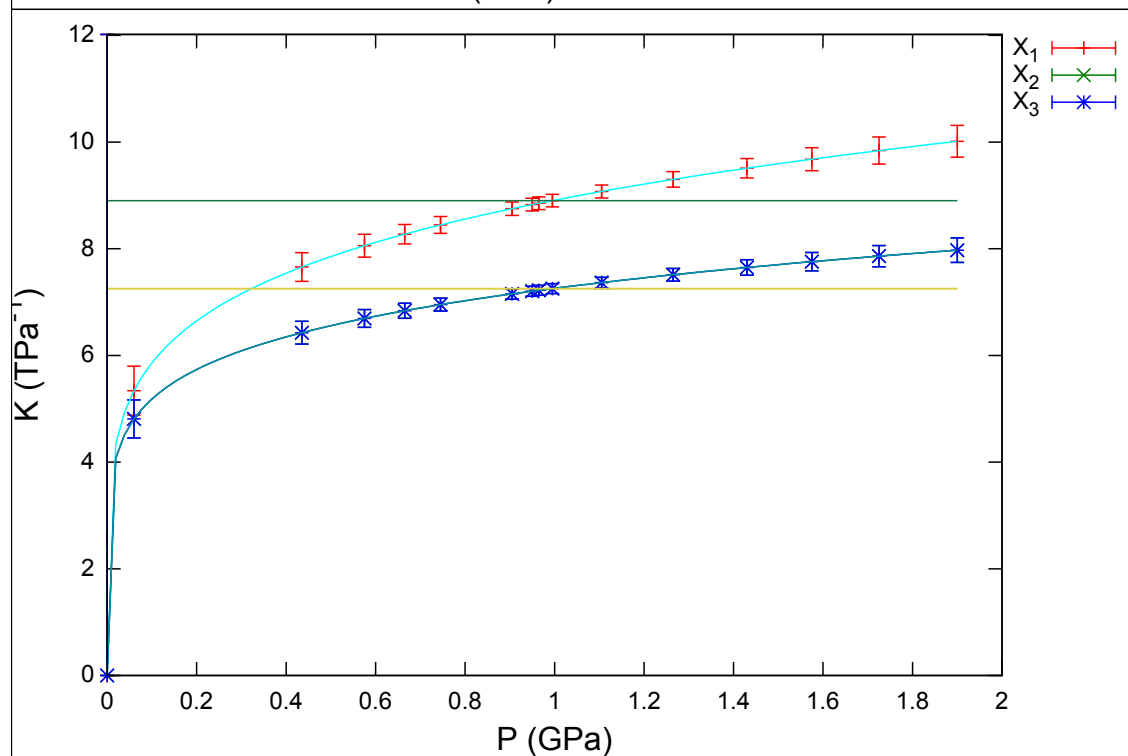
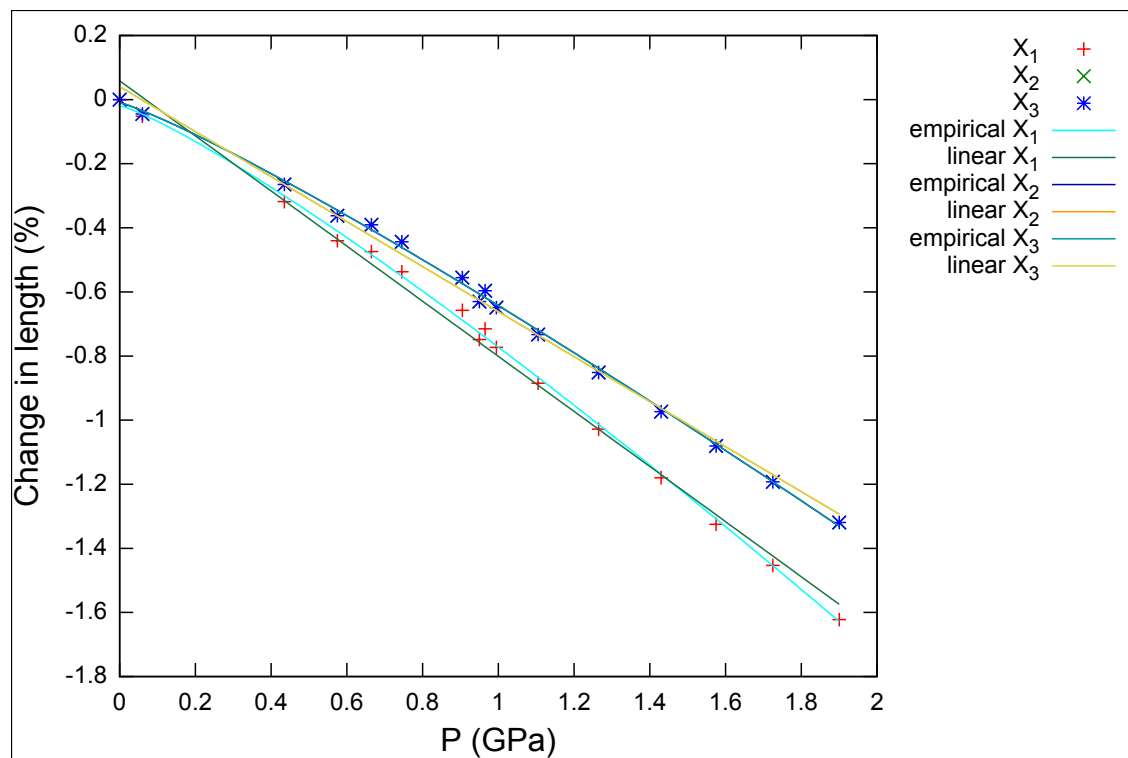
Down e_{33}

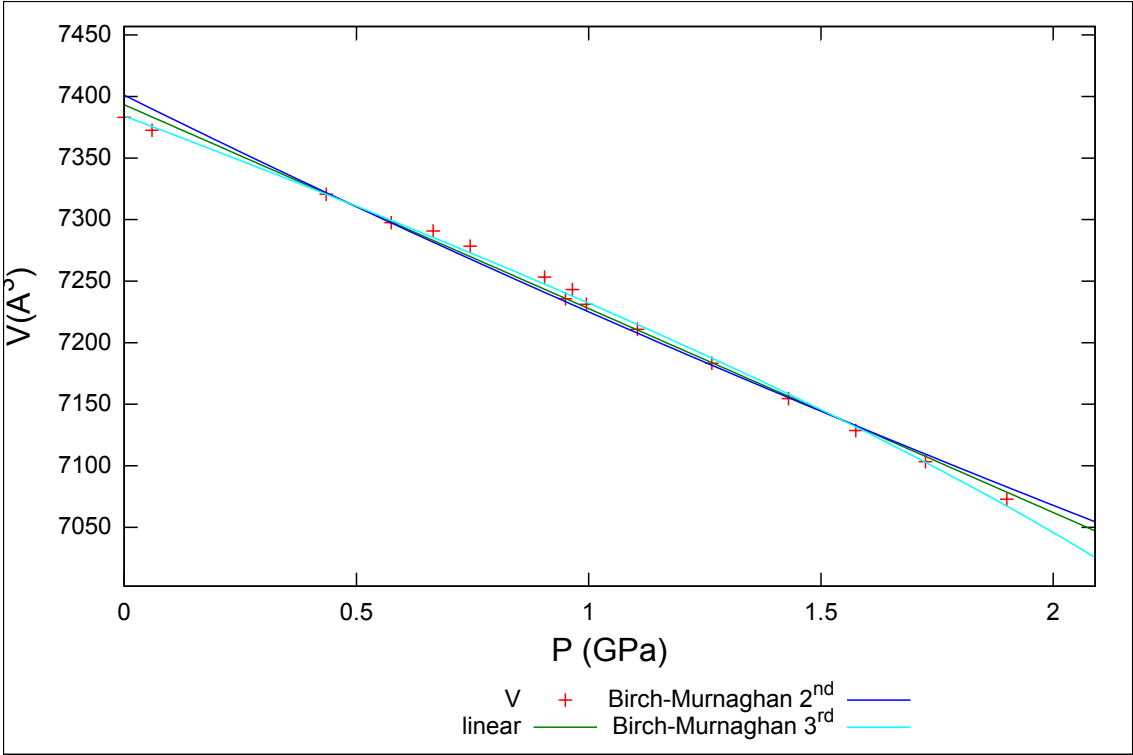
Value X:**30**

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	16548016036485063931592704.00	138910115475326511651749888.00	138910207568580369920819200.00
0.06	5.34	4.81	4.81	0.46	0.36	0.36
0.43	7.66	6.43	6.43	0.27	0.21	0.21
0.57	8.06	6.69	6.69	0.21	0.17	0.17
0.67	8.27	6.84	6.84	0.18	0.14	0.14
0.74	8.45	6.95	6.95	0.16	0.12	0.12
0.91	8.75	7.15	7.15	0.12	0.10	0.10
0.95	8.83	7.20	7.20	0.12	0.09	0.09
0.96	8.85	7.22	7.22	0.12	0.09	0.09
0.99	8.90	7.25	7.25	0.12	0.09	0.09
1.10	9.07	7.36	7.36	0.12	0.10	0.10
1.26	9.30	7.51	7.51	0.14	0.12	0.12
1.43	9.51	7.65	7.65	0.18	0.15	0.15
1.57	9.68	7.76	7.76	0.22	0.17	0.17
1.73	9.84	7.86	7.86	0.25	0.20	0.20
1.90	10.01	7.97	7.97	0.30	0.23	0.23

% 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	-0.0184	-0.0095	-0.0095
0.0600	-0.0516	-0.0447	-0.0447	-0.0455	-0.0347	-0.0347
0.4350	-0.3182	-0.2648	-0.2648	-0.3002	-0.2534	-0.2534
0.5750	-0.4401	-0.3622	-0.3622	-0.4103	-0.3453	-0.3453
0.6650	-0.4742	-0.3906	-0.3906	-0.4838	-0.4062	-0.4062
0.7450	-0.5371	-0.4437	-0.4437	-0.5507	-0.4613	-0.4613
0.9050	-0.6576	-0.5554	-0.5554	-0.6884	-0.5742	-0.5742
0.9500	-0.7486	-0.6304	-0.6304	-0.7279	-0.6065	-0.6065
0.9650	-0.7151	-0.5962	-0.5962	-0.7412	-0.6173	-0.6173
0.9950	-0.7728	-0.6491	-0.6491	-0.7678	-0.6391	-0.6391
1.1050	-0.8846	-0.7332	-0.7332	-0.8667	-0.7195	-0.7195
1.2650	-1.0283	-0.8513	-0.8513	-1.0137	-0.8385	-0.8385
1.4300	-1.1800	-0.9737	-0.9737	-1.1689	-0.9636	-0.9636
1.5750	-1.3250	-1.0805	-1.0805	-1.3080	-1.0753	-1.0753
1.7250	-1.4534	-1.1926	-1.1926	-1.4544	-1.1924	-1.1924
1.9000	-1.6225	-1.3196	-1.3196	-1.6282	-1.3310	-1.3310

Volume

P	P_{lin}	P_{calc,2nd}	P_{3rd}	V (Å³)
0.0000	0.0621	0.0970	0.0078	7383.0633
0.0600	0.1249	0.1536	0.0806	7372.6512
0.4350	0.4388	0.4422	0.4349	7320.6490
0.5750	0.5791	0.5744	0.5881	7297.4152
0.6650	0.6192	0.6127	0.6313	7290.7639
0.7450	0.6939	0.6843	0.7110	7278.3887
0.9050	0.8455	0.8315	0.8698	7253.2695
0.9500	0.9516	0.9360	0.9783	7235.7016
0.9650	0.9068	0.8918	0.9328	7243.1151
0.9950	0.9787	0.9629	1.0057	7231.2135
1.1050	1.1017	1.0861	1.1282	7210.8360
1.2650	1.2681	1.2554	1.2892	7183.2647
1.4300	1.4414	1.4352	1.4507	7154.5572
1.5750	1.5977	1.6004	1.5908	7128.6480
1.7250	1.7511	1.7653	1.7227	7103.2462
1.9000	1.9345	1.9664	1.8731	7072.8505

Input

P	σP	a	b	c	α	β	γ
0	0.1	17.351316	17.351316	28.316601	90	90	120
0.06	0.1	17.343553	17.343553	28.301986	90	90	120
0.435	0.1	17.305372	17.305372	28.226503	90	90	120
0.575	0.1	17.288467	17.288467	28.191972	90	90	120
0.665	0.1	17.283548	17.283548	28.182311	90	90	120
0.745	0.1	17.274332	17.274332	28.164503	90	90	120
0.905	0.1	17.254951	17.254951	28.130388	90	90	120
0.965	0.1	17.247863	17.247863	28.114099	90	90	120
0.95	0.1	17.241939	17.241939	28.104626	90	90	120
0.995	0.1	17.238692	17.238692	28.097775	90	90	120
1.105	0.1	17.224096	17.224096	28.066103	90	90	120
1.265	0.1	17.203604	17.203604	28.025435	90	90	120
1.43	0.1	17.182368	17.182368	27.982473	90	90	120
1.575	0.1	17.163829	17.163829	27.941401	90	90	120
1.725	0.1	17.144381	17.144381	27.905038	90	90	120
1.9	0.1	17.12235	17.12235	27.857177	90	90	120