

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	10.4705	0.3866	1.0000	-0.0000	-0.0000	3.5782e-04	-1.0865e-02	0.0000	0.8899
X_2	10.4705	0.3866	0.0000	1.0000	-0.0000	3.5782e-04	-1.0865e-02	0.0000	0.8899
X_3	10.4705	0.3866	0.0000	0.0000	1.0000	3.5782e-04	-1.0865e-02	0.0000	0.8899
V	31.2013	0.6240							

Birch-Murnaghan Coefficients

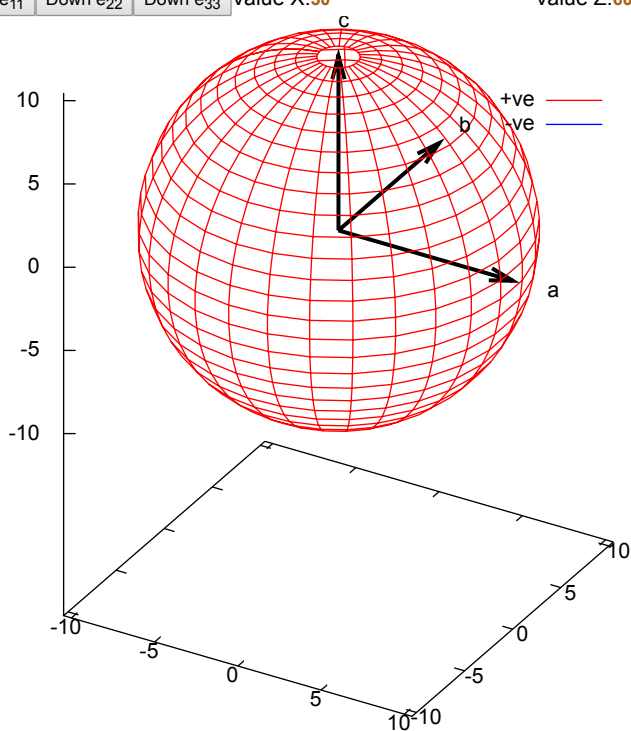
	B_0 (GPa)	σB_0 (GPa)	V_0 (\AA^3)	σV_0 (\AA^3)	B'	$\sigma B'$	P_c (GPa)
2 nd	29.3801	0.7806	3392.6600	1.6980	4	n/a	0
3 rd	25.5330	3.2091	3395.0588	2.8719	11.9430	7.0810	0

Compressibility Indicatrix

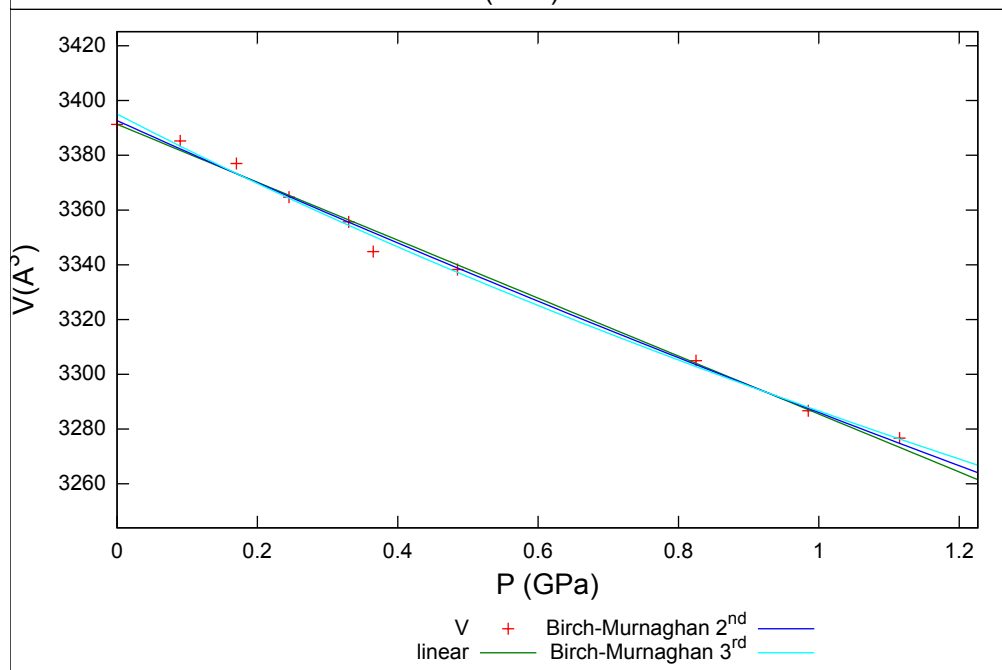
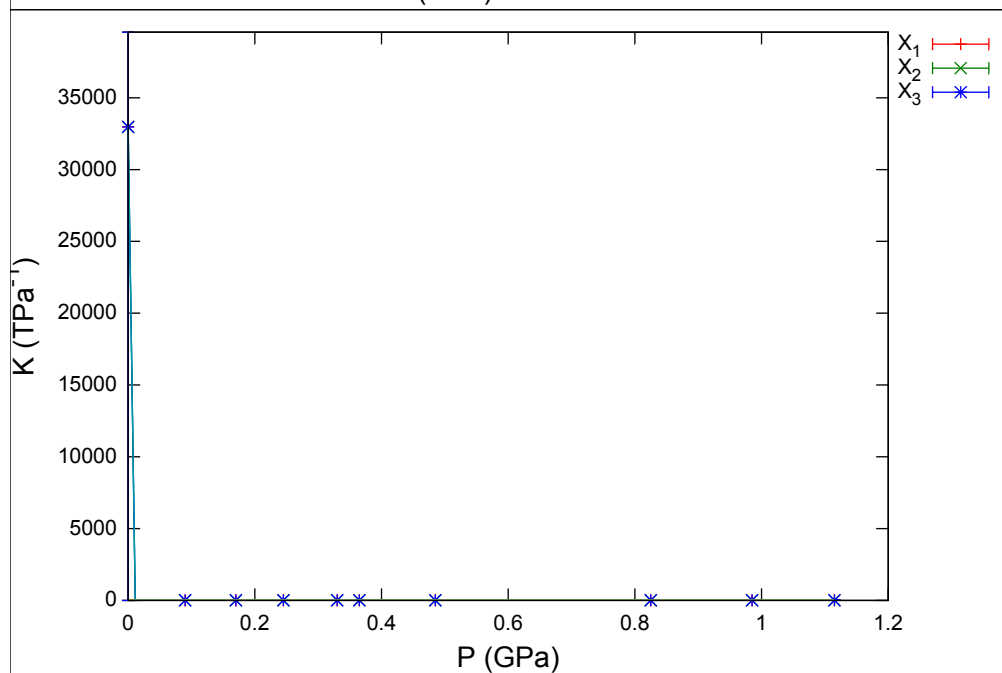
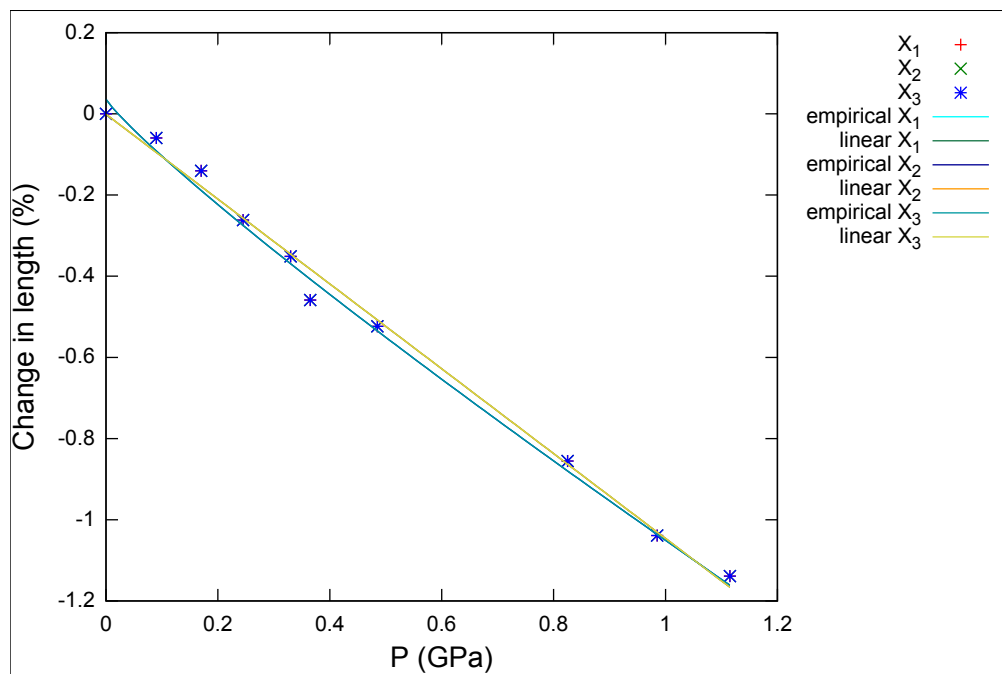
The compressibility indicatrix has units of TPa^{-1} .

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)

2/9/2018					PASCal				
P	K ₁	K ₂	K ₃	σK_1	σK_2	σK_3			
0.00	32975.23	32975.23	32975.25	11732620935029715062146782461952.00	11732620935029715062146782461952.00	11732621617911591661641			
0.09	12.60	12.60	12.60	2.89	2.89	2.89			
0.17	11.75	11.75	11.75	1.75	1.75	1.75			
0.24	11.29	11.29	11.29	1.18	1.18	1.18			
0.33	10.92	10.92	10.92	0.76	0.76	0.76			
0.36	10.80	10.80	10.80	0.63	0.63	0.63			
0.48	10.47	10.47	10.47	0.39	0.39	0.39			
0.82	9.88	9.88	9.88	0.67	0.67	0.67			
0.98	9.69	9.69	9.69	0.86	0.86	0.86			
1.11	9.55	9.55	9.55	0.99	0.99	0.99			

% 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	0.0358	0.0358	0.0358
0.0900	-0.0594	-0.0594	-0.0594	-0.0917	-0.0917	-0.0917
0.1700	-0.1405	-0.1405	-0.1405	-0.1887	-0.1887	-0.1887
0.2450	-0.2618	-0.2618	-0.2618	-0.2750	-0.2750	-0.2750
0.3300	-0.3511	-0.3511	-0.3511	-0.3693	-0.3693	-0.3693
0.3650	-0.4586	-0.4586	-0.4586	-0.4073	-0.4073	-0.4073
0.4850	-0.5234	-0.5234	-0.5234	-0.5348	-0.5348	-0.5348
0.8250	-0.8553	-0.8553	-0.8553	-0.8797	-0.8797	-0.8797
0.9850	-1.0388	-1.0388	-1.0388	-1.0362	-1.0362	-1.0362
1.1150	-1.1390	-1.1390	-1.1390	-1.1612	-1.1612	-1.1612

Volume

P	P _{lin}	P _{calc,2nd}	P _{3rd}	V (Å ³)
0.0000	0.0004	0.0121	0.0288	3391.2605
0.0900	0.0575	0.0648	0.0754	3385.2203
0.1700	0.1353	0.1373	0.1407	3376.9862
0.2450	0.2515	0.2472	0.2419	3364.6958
0.3300	0.3368	0.3293	0.3192	3355.6672
0.3650	0.4394	0.4293	0.4155	3344.8160
0.4850	0.5011	0.4903	0.4754	3338.2850
0.8250	0.8158	0.8106	0.8026	3304.9814
0.9850	0.9889	0.9936	0.9991	3286.6725
1.1150	1.0832	1.0954	1.1114	3276.6966

Input

P	σP	a	b	c	α	β	γ
0	0.1	15.024051	15.024051	15.024051	90	90	90
0.09	0.1	15.015126	15.015126	15.015126	90	90	90
0.17	0.1	15.002942	15.002942	15.002942	90	90	90
0.245	0.1	14.984719	14.984719	14.984719	90	90	90
0.33	0.1	14.971304	14.971304	14.971304	90	90	90
0.365	0.1	14.955149	14.955149	14.955149	90	90	90
0.485	0.1	14.945409	14.945409	14.945409	90	90	90
0.825	0.1	14.895543	14.895543	14.895543	90	90	90
0.985	0.1	14.867986	14.867986	14.867986	90	90	90
1.115	0.1	14.852928	14.852928	14.852928	90	90	90