

Output

4 data points entered - at least as many data points as parameters are needed for a fit to be carried out (i.e. 3 for 3rd order Birch-Murnaghan,4 for empirical pressure fitting). As PASCAL calculates errors from derivatives, more data points than parameters are needed for error estimates.

			Direction		
Axes	α (MK ⁻¹)	$\sigma\alpha$ (MK ⁻¹)	a	b	c
X₁	-2.8501	1.3244	-0.9688	0.0000	-0.2477
X₂	33.0661	2.9608	-0.1747	-0.0000	0.9846
X₃	36.6217	3.2541	0.0000	-1.0000	-0.0000
V	70.4313	6.8164			

% change in length

T	X_1	X_2	X_3	$X_{1,calc}$	$X_{2,calc}$	$X_{3,calc}$
30.0000	0.0000	0.0000	0.0000	-0.0066	-0.0167	-0.0141
50.0000	-0.0169	0.0340	0.0529	-0.0123	0.0494	0.0591
75.0000	-0.0287	0.1164	0.1236	-0.0194	0.1321	0.1507
100.0000	-0.0192	0.2293	0.2614	-0.0265	0.2148	0.2422

Volume

T	V (Å ³)	V _{lin} (Å ³)
30.0000	2746.6098	2745.2532
50.0000	2748.5317	2749.1221
75.0000	2752.4128	2753.9583
100.0000	2759.5738	2758.7945

Input

T	σT	a	b	c	α	β	γ
100	2	10.809	15.7339	17.0294	90	107.666	90
75	2	10.8076	15.7173	17.0045	90	107.657	90
50	2	10.8072	15.7062	16.9907	90	107.631	90
30	2	10.8082	15.6979	16.985	90	107.618	90