

Output

3 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	$\alpha(\text{MK}^{-1})$	$\sigma\alpha(\text{MK}^{-1})$	a	b	c
X_1	-31.7163	0.7437	0.9073	-0.0000	0.4205
X_2	36.7760	4.9933	0.0000	-1.0000	0.0000
X_3	114.0151	8.3832	-0.7858	0.0000	0.6185
V	129.5904	15.3968			

% change in length

T	X_1	X_2	X_3	$X_{1,\text{calc}}$	$X_{2,\text{calc}}$	$X_{3,\text{calc}}$
12.0000	0.0000	0.0000	0.0000	-0.0053	-0.0353	-0.0593
50.0000	-0.1350	0.0423	0.2696	-0.1258	0.1044	0.3740
100.0000	-0.2804	0.3152	0.9891	-0.2844	0.2883	0.9441

Volume

T	V (\AA^3)	V _{lin} (\AA^3)
12.0000	4652.7351	4646.0878
50.0000	4660.9690	4668.9999
100.0000	4700.5309	4699.1474

Input

T	σT	a	b	c	α	β	γ
12	2	11.3256	21.5132	19.1574	90	94.589	90
50	2	11.3291	21.5223	19.1834	90	94.812	90
100	2	11.3653	21.581	19.2469	90	95.308	90