

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	$\alpha(\text{MK}^{-1})$	$\sigma\alpha(\text{MK}^{-1})$	a	b	c
X_1	3.7799	2.5592	0.0000	-1.0000	0.0000
X_2	42.6172	6.8308	0.9478	-0.0000	0.3189
X_3	113.4662	4.9676	-0.0710	-0.0000	0.9975
V	160.9352	5.5050			

% change in length

T	X_1	X_2	X_3	$X_{1,\text{calc}}$	$X_{2,\text{calc}}$	$X_{3,\text{calc}}$
120.0000	0.0000	0.0000	0.0000	-0.0017	-0.0166	0.0039
130.0000	0.0057	0.0067	0.1114	0.0021	0.0261	0.1174
140.0000	-0.0067	0.0577	0.2546	0.0058	0.0687	0.2309
150.0000	0.0167	0.1251	0.3305	0.0096	0.1113	0.3443

Volume

T	V (\AA^3)	V _{lin} (\AA^3)
120.0000	3722.6310	3722.0430
130.0000	3727.2425	3728.0341
140.0000	3734.0143	3734.0251
150.0000	3740.2305	3740.0161

Input

T	σT	a	b	c	α	β	γ
120	2	19.7604	11.9415	16.071	90	100.996	90
130	2	19.7618	11.9423	16.0888	90	100.998	90
140	2	19.7747	11.9407	16.1117	90	101.035	90
150	2	19.7876	11.9435	16.124	90	101.031	90