

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	23.1610	0.2629	-0.9903	-0.0000	-0.1389	
X_2	26.7161	0.2476	-0.0000	1.0000	-0.0000	
X_3	75.2159	0.8554	0.1084	-0.0000	0.9941	
V	125.4639	0.9150				

% change in length

T	X_1	X_2	X_3	$X_{1,\text{calc}}$	$X_{2,\text{calc}}$	$X_{3,\text{calc}}$
225.0000	0.0000	0.0000	0.0000	-0.0002	0.0017	0.0052
250.0000	0.0592	0.0717	0.1992	0.0577	0.0685	0.1932
275.0000	0.1122	0.1340	0.3847	0.1156	0.1353	0.3812
300.0000	0.1753	0.2019	0.5650	0.1735	0.2021	0.5693

Volume

T	V (\AA^3)	V _{lin} (\AA^3)
225.0000	2851.3638	2851.5430
250.0000	2860.7852	2860.4865
275.0000	2869.3847	2869.4301
300.0000	2878.2996	2878.3737

Input

T	σT	a	b	c	α	β	γ
300	2	10.8097	15.9326	17.4617	90	106.847	90
275	2	10.8017	15.9218	17.4303	90	106.825	90
250	2	10.7949	15.9119	17.3979	90	106.804	90
225	2	10.7881	15.9005	17.3637	90	106.801	90