

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	-5.4190	6.2249	0.0000	1.0000	-0.0000
X_2	29.7533	1.1705	-0.6348	0.0000	0.7726
X_3	65.6308	0.6124	0.9320	-0.0000	0.3625
V	93.1848	7.0619			

% change in length

T	X_1	X_2	X_3	$X_{1,\text{calc}}$	$X_{2,\text{calc}}$	$X_{3,\text{calc}}$
80.0000	0.0000	0.0000	0.0000	-0.0176	-0.0033	0.0017
130.0000	-0.1063	0.1339	0.3359	-0.0447	0.1455	0.3299
150.0000	-0.0115	0.2132	0.4568	-0.0555	0.2050	0.4611

Volume

T	V (\AA^3)	V _{lin} (\AA^3)
80.0000	2907.6448	2906.7223
130.0000	2918.2145	2920.2698
150.0000	2926.8215	2925.6887

Input

T	σT	a	b	c	α	β	γ
80	2	10.1545	19.0923	15.0033	90	91.566	90
130	2	10.1834	19.072	15.0304	90	91.467	90
150	2	10.1952	19.0901	15.0429	90	91.451	90