

Output

2 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	$\alpha$ (MK <sup>-1</sup> )	$\sigma\alpha$ (MK <sup>-1</sup> )	a	b	c	
X <sub>1</sub>	54.9700	0.0000	-0.3117	0.0000	-0.9502	
X <sub>2</sub>	75.3140	0.0000	0.0000	1.0000	-0.0000	
X <sub>3</sub>	111.8588	0.0000	-0.9899	0.0000	0.1418	
V	242.5203	0.0000				

% change in length

T	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>1,calc</sub>	X <sub>2,calc</sub>	X <sub>3,calc</sub>
310.0000	0.0000	0.0000	0.0000	-0.0000	-0.0000	-0.0000
330.0000	0.1099	0.1506	0.2237	0.1099	0.1506	0.2237

Volume

T	V (Å <sup>3</sup> )	V <sub>lin</sub> (Å <sup>3</sup> )
310.0000	3144.8762	3144.8762
330.0000	3160.1302	3160.1302

Input

T	$\sigma T$	a	b	c	$\alpha$	$\beta$	$\gamma$
310	2	10.6308	19.4519	15.213	90	91.451	90
330	2	10.6541	19.4812	15.2306	90	91.478	90