

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	$\alpha$ (MK <sup>-1</sup> )	$\sigma\alpha$ (MK <sup>-1</sup> )	a	b	c	
X <sub>1</sub>	-20.0977	1.1420	0.9763	-0.0000	0.2164	
X <sub>2</sub>	27.4023	2.6962	0.0112	-0.0000	0.9999	
X <sub>3</sub>	67.4595	2.4641	-0.0000	1.0000	-0.0000	
V	77.3617	5.5343				

% 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>
90.0000	0.0000	0.0000	0.0000	0.0022	-0.0051	-0.0037
110.0000	-0.0289	0.0450	0.1299	-0.0380	0.0497	0.1312
120.0000	-0.0676	0.0659	0.1861	-0.0581	0.0771	0.1986
130.0000	-0.0757	0.1152	0.2761	-0.0782	0.1045	0.2661

Volume

T	V (Å <sup>3</sup> )	V <sub>lin</sub> (Å <sup>3</sup> )
90.0000	1005.1808	1005.0546
110.0000	1006.6485	1006.6099
120.0000	1007.0343	1007.3875
130.0000	1008.3536	1008.1651

Input

T	$\sigma$ T	a	b	c	$\alpha$	$\beta$	$\gamma$
130	2	10.1637	8.0269	12.9143	90	106.85	90
120	2	10.1634	8.0197	12.9080	90	106.83	90
110	2	10.1668	8.0152	12.9053	90	106.82	90
90	2	10.1692	8.0048	12.8995	90	106.81	90