

Output

Axes	$\alpha$ (MK <sup>-1</sup> )	$\sigma\alpha$ (MK <sup>-1</sup> )	Direction		
			a	b	c
X <sub>1</sub>	9.9373	5.4575	0.8353	-0.0000	-0.5497
X <sub>2</sub>	60.8956	1.6931	0.0000	-1.0000	0.0000
X <sub>3</sub>	153.1649	8.6500	0.8806	-0.0000	0.4739
V	227.7651	4.0904			

% 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>
125.0000	0.0000	0.0000	0.0000	-0.0149	0.0248	-0.1023
130.0000	-0.1335	0.0028	0.0384	-0.0099	0.0553	-0.0257
143.0000	-0.0699	0.1494	0.2746	0.0030	0.1344	0.1734
165.0000	0.1469	0.3557	0.3672	0.0249	0.2684	0.5104
200.0000	0.1949	0.4731	0.7902	0.0597	0.4815	1.0465
298.0000	0.0813	1.0617	2.6793	0.1570	1.0783	2.5475

Volume

T	V (Å <sup>3</sup> )	V <sub>lin</sub> (Å <sup>3</sup> )
125.0000	4800.1811	4795.2748
130.0000	4795.7509	4800.7414
143.0000	4817.2022	4814.9545
165.0000	4842.0562	4839.0074
200.0000	4870.5143	4877.2733
298.0000	4985.9648	4984.4181

Input

T	$\sigma$ T	a	b	c	$\alpha$	$\beta$	$\gamma$
125	2	11.4182	21.8134	19.3128	90	93.705	90
130	2	11.4090	21.814	19.308	90	93.612	90
143	2	11.426	21.846	19.335	90	93.51	90
165	2	11.448	21.891	19.359	90	93.58	90
200	2	11.4725	21.9166	19.4189	90	94.041	90
298	2	11.571	22.045	19.626	90	95.16	90