

Output

Axes			Direction		
	$\alpha$ (MK <sup>-1</sup> )	$\sigma\alpha$ (MK <sup>-1</sup> )	a	b	c
X <sub>1</sub>	-1.3614	8.0937	-0.8527	0.0000	-0.5224
X <sub>2</sub>	53.9409	8.1432	-0.6308	-0.0000	0.7759
X <sub>3</sub>	54.9704	2.8472	0.0000	-1.0000	-0.0000
V	123.3405	22.3558			

% 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>
200.0000	0.0000	0.0000	0.0000	-0.0881	-0.0904	-0.0190
220.0000	-0.2060	-0.0883	0.0366	-0.0908	0.0175	0.0910
240.0000	-0.0914	0.1195	0.2268	-0.0935	0.1254	0.2009
260.0000	-0.0897	0.2291	0.3366	-0.0962	0.2333	0.3109
280.0000	-0.0979	0.3384	0.4146	-0.0990	0.3412	0.4208
300.0000	-0.0843	0.4773	0.5209	-0.1017	0.4490	0.5308

Volume

T	V (Å <sup>3</sup> )	V <sub>lin</sub> (Å <sup>3</sup> )
200.0000	1061.2218	1058.2958
220.0000	1058.4883	1060.9137
240.0000	1063.9267	1063.5315
260.0000	1066.2780	1066.1493
280.0000	1068.1837	1068.7672
300.0000	1070.9440	1071.3850

Input

T	$\sigma$ T	a	b	c	$\alpha$	$\beta$	$\gamma$
300	2	10.152	8.511	13.1826	90	109.910	90
280	2	10.141	8.502	13.171	90	109.840	90
260	2	10.1332	8.4954	13.1623	90	109.773	90
240	2	10.1252	8.4861	13.1527	90	109.708	90
220	2	10.1062	8.4700	13.1286	90	109.63	90
200	2	10.1258	8.4669	13.1402	90	109.61	90