

Output

			Direction		
Axes	α (MK ⁻¹)	$\sigma\alpha$ (MK ⁻¹)	a	b	c
X ₁	-36.2651	5.0980	0.8175	0.5759	-0.0000
X ₂	-36.2651	5.0980	-0.3009	0.9536	-0.0000
X ₃	375.8687	15.4252	-0.0000	-0.0000	1.0000
V	301.3925	5.6432			

% change in length

T	X ₁	X ₂	X ₃	X _{1,calc}	X _{2,calc}	X _{3,calc}
140.0000	0.0000	0.0000	0.0000	0.1776	0.1776	-0.4827
150.0000	0.0734	0.0734	0.1221	0.1413	0.1413	-0.1068
160.0000	0.1194	0.1194	0.2912	0.1051	0.1051	0.2690
180.0000	0.1377	0.1377	0.7576	0.0326	0.0326	1.0208
200.0000	0.1010	0.1010	1.3619	-0.0400	-0.0400	1.7725
220.0000	0.0009	0.0009	2.1414	-0.1125	-0.1125	2.5243
240.0000	-0.1331	-0.1331	3.0431	-0.1850	-0.1850	3.2760
260.0000	-0.2782	-0.2782	3.9636	-0.2576	-0.2576	4.0277
280.0000	-0.3764	-0.3764	4.9623	-0.3301	-0.3301	4.7795
290.0000	-0.4214	-0.4214	5.3035	-0.3664	-0.3664	5.1553
300.0000	-0.4609	-0.4609	5.8201	-0.4026	-0.4026	5.5312

Volume

T	V (Å ³)	V _{lin} (Å ³)
140.0000	3281.6662	3277.5374
150.0000	3290.5015	3287.4281
160.0000	3299.0822	3297.3188
180.0000	3315.6432	3317.1002
200.0000	3333.0808	3336.8816
220.0000	3352.0029	3356.6630
240.0000	3372.5336	3376.4444
260.0000	3392.7814	3396.2258
280.0000	3418.6284	3416.0071
290.0000	3426.6462	3425.8978
300.0000	3440.7262	3435.7885

Input

T	σ T	a	b	c	α	β	γ
140	2	10.892	10.892	31.941	90	90	120
150	2	10.9	10.9	31.98	90	90	120
160	2	10.905	10.905	32.034	90	90	120
180	2	10.907	10.907	32.183	90	90	120
200	2	10.903	10.903	32.376	90	90	120
220	2	10.8921	10.8921	32.625	90	90	120
240	2	10.8775	10.8775	32.913	90	90	120
260	2	10.8617	10.8617	33.207	90	90	120
280	2	10.851	10.851	33.526	90	90	120
290	2	10.8461	10.8461	33.635	90	90	120
300	2	10.8418	10.8418	33.8	90	90	120