

Output

Axes			Direction		
	α (MK ⁻¹)	$\sigma\alpha$ (MK ⁻¹)	a	b	c
X ₁	-19.1133	0.8356	0.9322	-0.0000	0.3620
X ₂	64.7062	1.1860	-0.0000	-1.0000	-0.0000
X ₃	173.7229	1.4726	-0.1125	-0.0000	0.9936
V	219.8289	0.5458			

% change in length

T	X ₁	X ₂	X ₃	X _{1,calc}	X _{2,calc}	X _{3,calc}
165.0000	0.0000	0.0000	0.0000	0.0063	0.0009	-0.0092
170.0000	-0.0015	0.0259	0.0854	-0.0032	0.0332	0.0777
180.0000	-0.0153	0.0895	0.2496	-0.0223	0.0979	0.2514
190.0000	-0.0457	0.1715	0.4072	-0.0414	0.1626	0.4251
200.0000	-0.0588	0.2426	0.5942	-0.0606	0.2273	0.5988
210.0000	-0.0780	0.2987	0.7656	-0.0797	0.2920	0.7726
220.0000	-0.0945	0.3531	0.9481	-0.0988	0.3567	0.9463
230.0000	-0.1238	0.4108	1.1324	-0.1179	0.4214	1.1200

Volume

T	V (Å ³)	V _{lin} (Å ³)
165.0000	3759.8728	3759.7788
170.0000	3764.0042	3763.9115
180.0000	3772.0540	3772.1768
190.0000	3779.9336	3780.4421
200.0000	3789.1626	3788.7073
210.0000	3797.0166	3796.9726
220.0000	3805.3296	3805.2379
230.0000	3813.3570	3813.5032

Input

T	σ T	a	b	c	α	β	γ
230	2	20.1794	12.0018	15.9842	90	99.917	90
220	2	20.1813	11.9949	15.9557	90	99.865	90
210	2	20.1805	11.9884	15.9276	90	99.813	90
200	2	20.1813	11.9817	15.9009	90	99.771	90
190	2	20.1809	11.9732	15.8717	90	99.728	90
180	2	20.1826	11.9634	15.8477	90	99.674	90
170	2	20.1826	11.9558	15.8221	90	99.635	90
165	2	20.1812	11.9527	15.8089	90	99.613	90