Output

			Direction		
Axes	$\alpha(MK^{-1})$	$\sigma\alpha\ (MK^{-1})$	a	b	c
X_1	20.7497	2.1875	0.9172	-0.0000	-0.3983
X_2	56.2551	2.1169	0.0000	-1.0000	0.0000
X_3	73.3810	2.5387	0.9025	-0.0000	0.4307
V	152.4510	4.4908			

% change in length

T	X_1	X_2	X_3	$X_{1,calc}$	$X_{2,calc}$	$X_{3,calc}$
100.0000	0.0000	0.0000	0.0000	-0.0215	-0.0210	-0.0021
110.0000	0.0108	0.0518	0.0567	-0.0007	0.0353	0.0713
120.0000	0.0404	0.1070	0.1107	0.0200	0.0915	0.1447
130.0000	0.0157	0.1084	0.2574	0.0408	0.1478	0.2180
140.0000	0.0226	0.1767	0.3074	0.0615	0.2040	0.2914
150.0000	0.0622	0.2415	0.3574	0.0823	0.2603	0.3648
160.0000	0.0920	0.3063	0.4263	0.1030	0.3165	0.4382
170.0000	0.1396	0.3993	0.5585	0.1238	0.3728	0.5116
180.0000	0.1429	0.4252	0.5759	0.1445	0.4290	0.5849
190.0000	0.1927	0.5053	0.6308	0.1653	0.4853	0.6583

Volume

T	V ($Å^3$)	V_{lin} ($Å^3$)
100.0000	1305.1805	1304.5028
110.0000	1306.7382	1306.4926
120.0000	1308.5517	1308.4823
130.0000	1310.1658	1310.4721
140.0000	1311.8053	1312.4619
150.0000	1313.8272	1314.4516
160.0000	1315.9712	1316.4414
170.0000	1319.5560	1318.4311
180.0000	1320.1704	1320.4209
190.0000	1322.6011	1322.4107

Input

T	σT	a	b	c	α	β	γ
190	2	8.4636	8.5322	18.4815	90	97.691	90
180	2	8.4591	8.5254	18.4722	90	97.694	90
170	2	8.4578	8.5232	18.4716	90	97.703	90
160	2	8.4527	8.5153	18.4516	90	97.748	90
150	2	8.4489	8.5098	18.4427	90	97.77	90
140	2	8.445	8.5043	18.435	90	97.776	90
130	2	8.4424	8.4985	18.4313	90	97.801	90
120	2	8.4399	8.4987	18.418	90	97.9	90
110	2	8.436	8.4937	18.4123	90	97.911	90
100	2	8.4335	8.4893	18.4065	90	97.937	90