

Output

			Direction		
Axes	$\alpha(\text{MK}^{-1})$	$\sigma\alpha(\text{MK}^{-1})$	a	b	c
X ₁	29.3991	1.6053	-0.9224	-0.0000	0.3861
X ₂	60.1261	1.6215	0.0000	1.0000	0.0000
X ₃	77.7991	2.1907	-0.8975	0.0000	-0.4410
V	169.9732	5.2543			

% 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	-0.0225	-0.0337	-0.0466
110.0000	-0.0074	0.0216	0.0318	0.0069	0.0264	0.0312
120.0000	0.0553	0.0941	0.1100	0.0363	0.0865	0.1090
130.0000	0.0677	0.1470	0.1820	0.0657	0.1466	0.1868
140.0000	0.1121	0.2105	0.2630	0.0951	0.2068	0.2646
150.0000	0.0969	0.2494	0.3354	0.1245	0.2669	0.3424
160.0000	0.1352	0.2964	0.3656	0.1539	0.3270	0.4202
170.0000	0.1713	0.3658	0.4831	0.1833	0.3871	0.4980
180.0000	0.2070	0.4434	0.5697	0.2127	0.4473	0.5758
190.0000	0.2170	0.4799	0.6335	0.2421	0.5074	0.6536
200.0000	0.2676	0.5834	0.7235	0.2715	0.5675	0.7314
210.0000	0.3117	0.6458	0.8395	0.3009	0.6277	0.8092
220.0000	0.3656	0.7140	0.9251	0.3303	0.6878	0.8870

Volume

T	V (Å ³)	V _{lin} (Å ³)
100.0000	1303.7275	1302.2310
110.0000	1304.3262	1304.4470
120.0000	1307.1129	1306.6630
130.0000	1308.9065	1308.8790
140.0000	1311.3774	1311.0950
150.0000	1312.6339	1313.3110
160.0000	1314.1496	1315.5270
170.0000	1317.0736	1317.7430
180.0000	1319.6998	1319.9590
190.0000	1321.1489	1322.1749
200.0000	1324.3614	1324.3909
210.0000	1327.2948	1326.6069
220.0000	1330.0383	1328.8229

Input

T	σT	a	b	c	α	β	γ
220	2	8.4807	8.5624	18.4814	90	97.665	90
210	2	8.4767	8.5566	18.4654	90	97.686	90
200	2	8.4734	8.5513	18.4455	90	97.739	90
190	2	8.4617	8.5425	18.4454	90	97.744	90
180	2	8.4582	8.5394	18.4408	90	97.774	90
170	2	8.4546	8.5328	18.4275	90	97.804	90
160	2	8.4462	8.5269	18.4196	90	97.849	90
150	2	8.4438	8.5229	18.4120	90	97.844	90
140	2	8.4428	8.5196	18.4059	90	97.894	90
130	2	8.4378	8.5142	18.3947	90	97.915	90
120	2	8.4338	8.5097	18.3894	90	97.948	90
110	2	8.4289	8.5044	18.3741	90	97.988	90
100	2	8.4272	8.5017	18.3748	90	97.979	90