

Output

			Direction		
Axes	α (MK ⁻¹)	$\sigma\alpha$ (MK ⁻¹)	a	b	c
X ₁	7.0376	1.2053	-0.9618	0.0000	0.2738
X ₂	62.8805	1.4617	0.0000	1.0000	-0.0000
X ₃	126.7058	4.7530	0.8414	-0.0000	0.5404
V	204.4818	7.2775			

% 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	-0.0125	-0.0683	-0.2650
110.0000	0.0123	0.0521	0.0752	-0.0054	-0.0055	-0.1383
120.0000	0.0445	0.1125	0.1600	0.0016	0.0574	-0.0116
130.0000	0.0438	0.1244	0.1952	0.0087	0.1203	0.1151
140.0000	-0.0166	0.1789	0.2784	0.0157	0.1832	0.2418
150.0000	0.0339	0.2618	0.3947	0.0227	0.2461	0.3685
160.0000	0.0707	0.3175	0.4799	0.0298	0.3089	0.4952
170.0000	0.0870	0.3388	0.5509	0.0368	0.3718	0.6219
180.0000	-0.0020	0.4016	0.6346	0.0438	0.4347	0.7486
190.0000	0.1335	0.4359	0.7184	0.0509	0.4976	0.8753
200.0000	0.0701	0.5259	0.8592	0.0579	0.5605	1.0020
210.0000	0.0024	0.6207	0.9867	0.0650	0.6233	1.1287
220.0000	-0.0048	0.6716	1.1217	0.0720	0.6862	1.2554
230.0000	0.0076	0.7261	1.2434	0.0790	0.7491	1.3821
240.0000	0.0799	0.7889	1.3592	0.0861	0.8120	1.5088
250.0000	0.0450	0.8505	1.5415	0.0931	0.8749	1.6355
260.0000	0.0096	0.8789	1.6216	0.1001	0.9377	1.7623
270.0000	0.1035	0.9974	1.7963	0.1072	1.0006	1.8890
280.0000	0.0345	1.0033	1.8657	0.1142	1.0635	2.0157
290.0000	0.0673	1.0566	2.0350	0.1213	1.1264	2.1424
300.0000	0.1084	1.1301	2.2155	0.1283	1.1893	2.2691
310.0000	0.1829	1.3137	2.4822	0.1353	1.2521	2.3958
320.0000	0.2372	1.3350	2.6624	0.1424	1.3150	2.5225
330.0000	0.2184	1.4428	2.8327	0.1494	1.3779	2.6492
340.0000	0.2027	1.5234	2.9968	0.1564	1.4408	2.7759
350.0000	0.1917	1.5707	3.1811	0.1635	1.5037	2.9026

Volume

T	V (Å ³)	V _{lin} (Å ³)
100.0000	1325.3089	1319.7154
110.0000	1327.1603	1322.4254
120.0000	1329.5144	1325.1355
130.0000	1330.1302	1327.8455
140.0000	1331.1574	1330.5555
150.0000	1334.4793	1333.2655
160.0000	1336.8457	1335.9755
170.0000	1338.2932	1338.6855
180.0000	1339.0602	1341.3955
190.0000	1342.4492	1344.1056
200.0000	1344.6877	1346.8156
210.0000	1346.7556	1349.5256
220.0000	1349.1510	1352.2356
230.0000	1351.6800	1354.9456
240.0000	1355.0514	1357.6556
250.0000	1357.8635	1360.3656
260.0000	1358.8478	1363.0757
270.0000	1364.0704	1365.7857
280.0000	1364.1559	1368.4957
290.0000	1367.6074	1371.2057
300.0000	1371.6050	1373.9157
310.0000	1378.7325	1376.6257
320.0000	1382.2162	1379.3358

330.0000 1385.7521 1382.0458
340.0000 1388.8811 1384.7558
350.0000 1391.8994 1387.4658

Input

T	σT	a	b	c	α	β	γ
350	2	8.5273	8.5745	19.121	90	95.388	90
340	2	8.5219	8.5705	19.104	90	95.497	90
330	2	8.5180	8.5637	19.088	90	95.595	90
320	2	8.5148	8.5546	19.070	90	95.695	90
310	2	8.5050	8.5528	19.0504	90	95.771	90
300	2	8.4933	8.5373	19.016	90	95.875	90
290	2	8.4850	8.5311	18.9957	90	95.956	90
280	2	8.4789	8.5266	18.9739	90	96.028	90
270	2	8.4810	8.5261	18.9718	90	96.104	90
260	2	8.4708	8.5161	18.9457	90	96.148	90
250	2	8.4716	8.5137	18.9376	90	96.206	90
240	2	8.4701	8.5085	18.9173	90	96.317	90
230	2	8.4629	8.5032	18.8989	90	96.340	90
220	2	8.4591	8.4986	18.8844	90	96.399	90
210	2	8.4578	8.4943	18.8658	90	96.466	90
200	2	8.4569	8.4863	18.8610	90	96.583	90
190	2	8.4572	8.4787	18.8501	90	96.695	90
180	2	8.4483	8.4758	18.8273	90	96.657	90
170	2	8.4498	8.4705	18.8292	90	96.767	90
160	2	8.4480	8.4687	18.8177	90	96.789	90
150	2	8.4452	8.4640	18.8016	90	96.803	90
140	2	8.4400	8.4570	18.7831	90	96.834	90
130	2	8.4408	8.4524	18.7806	90	96.924	90
120	2	8.4401	8.4514	18.7766	90	96.947	90
110	2	8.4379	8.4463	18.7598	90	96.953	90
100	2	8.4358	8.4419	18.7493	90	96.984	90