

Output

			Direction		
Axes	α (MK ⁻¹)	$\sigma\alpha$ (MK ⁻¹)	a	b	c
X ₁	14.2102	1.4090	0.9483	-0.0000	-0.3174
X ₂	52.0557	0.8331	0.0000	-1.0000	0.0000
X ₃	97.9597	2.8477	0.8663	-0.0000	0.4996
V	167.8124	4.3816			

% 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	-0.0304	-0.0056	-0.1562
110.0000	0.0006	0.0577	0.0722	-0.0162	0.0464	-0.0582
120.0000	-0.0283	0.1059	0.1285	-0.0020	0.0985	0.0397
130.0000	-0.0020	0.1483	0.1963	0.0122	0.1505	0.1377
140.0000	0.0342	0.2059	0.2620	0.0264	0.2026	0.2356
150.0000	0.0228	0.2506	0.3728	0.0406	0.2546	0.3336
160.0000	0.0410	0.2930	0.3968	0.0548	0.3067	0.4316
170.0000	0.0406	0.3636	0.4952	0.0691	0.3587	0.5295
180.0000	0.0446	0.4001	0.5776	0.0833	0.4108	0.6275
190.0000	0.1012	0.4601	0.6536	0.0975	0.4629	0.7254
200.0000	0.1280	0.5130	0.7465	0.1117	0.5149	0.8234
210.0000	0.1496	0.5566	0.8199	0.1259	0.5670	0.9214
220.0000	0.2032	0.6083	0.9084	0.1401	0.6190	1.0193
230.0000	0.1673	0.6684	1.0306	0.1543	0.6711	1.1173
240.0000	0.1471	0.7554	1.1101	0.1685	0.7231	1.2152
250.0000	0.1885	0.7743	1.2284	0.1827	0.7752	1.3132
260.0000	0.1815	0.8190	1.3222	0.1969	0.8272	1.4112
270.0000	0.2039	0.8766	1.4224	0.2112	0.8793	1.5091
280.0000	0.2111	0.9225	1.5451	0.2254	0.9314	1.6071
290.0000	0.2341	1.0096	1.6909	0.2396	0.9834	1.7050
300.0000	0.2667	0.9731	1.7940	0.2538	1.0355	1.8030
310.0000	0.2919	1.0967	1.9247	0.2680	1.0875	1.9010
320.0000	0.2994	1.1661	2.0745	0.2822	1.1396	1.9989
330.0000	0.2763	1.1932	2.1874	0.2964	1.1916	2.0969
340.0000	0.4185	1.3132	2.3880	0.3106	1.2437	2.1948
350.0000	0.2060	1.2402	2.4282	0.3248	1.2957	2.2928

Volume

T	V (Å ³)	V _{lin} (Å ³)
100.0000	1319.4225	1316.5136
110.0000	1321.1438	1318.7278
120.0000	1322.1437	1320.9419
130.0000	1323.9468	1323.1561
140.0000	1326.0580	1325.3702
150.0000	1327.9671	1327.5844
160.0000	1329.0873	1329.7986
170.0000	1331.3237	1332.0127
180.0000	1332.9549	1334.2269
190.0000	1335.5172	1336.4410
200.0000	1337.8134	1338.6552
210.0000	1339.6599	1340.8693
220.0000	1342.2457	1343.0835
230.0000	1344.1983	1345.2976
240.0000	1346.1546	1347.5118
250.0000	1348.5434	1349.7259
260.0000	1350.3046	1351.9401
270.0000	1352.7211	1354.1542
280.0000	1355.0812	1356.3684
290.0000	1358.5206	1358.5826
300.0000	1359.8568	1360.7967
310.0000	1363.6205	1363.0109
320.0000	1366.6813	1365.2250

330.0000 1368.2597 1367.4392
340.0000 1374.5260 1369.6533
350.0000 1371.2024 1371.8675

Input

	T	σ T	a	b	c	α	β	γ
350	2	8.5233	8.6038	18.8098	90	96.240	90	
340	2	8.5345	8.6100	18.8221	90	96.378	90	
330	2	8.5172	8.5998	18.7982	90	96.421	90	
320	2	8.5167	8.5975	18.7852	90	96.490	90	
310	2	8.5116	8.5916	18.7702	90	96.569	90	
300	2	8.5098	8.5811	18.747	90	96.615	90	
290	2	8.5030	8.5842	18.7385	90	96.660	90	
280	2	8.4960	8.5768	18.7254	90	96.733	90	
270	2	8.4922	8.5729	18.7121	90	96.796	90	
260	2	8.4885	8.5680	18.6991	90	96.837	90	
250	2	8.4866	8.5642	18.6893	90	96.891	90	
240	2	8.4817	8.5626	18.6720	90	96.930	90	
230	2	8.4806	8.5552	18.6656	90	96.985	90	
220	2	8.4771	8.5501	18.6612	90	97.082	90	
210	2	8.4748	8.5457	18.6401	90	97.087	90	
200	2	8.4706	8.5420	18.6330	90	97.119	90	
190	2	8.4671	8.5375	18.6199	90	97.153	90	
180	2	8.4614	8.5324	18.6083	90	97.165	90	
170	2	8.4585	8.5293	18.6005	90	97.210	90	
160	2	8.4575	8.5233	18.5865	90	97.258	90	
150	2	8.4566	8.5197	18.5807	90	97.259	90	
140	2	8.4525	8.5159	18.5743	90	97.332	90	
130	2	8.4485	8.5110	18.5649	90	97.349	90	
120	2	8.4443	8.5074	18.5579	90	97.378	90	
110	2	8.4451	8.5033	18.5529	90	97.422	90	
100	2	8.4441	8.4984	18.5430	90	97.455	90	