

Output

Axes			Direction		
	α (MK ⁻¹)	$\sigma\alpha$ (MK ⁻¹)	a	b	c
X ₁	-3.1821	0.6430	-0.9549	0.0000	0.2968
X ₂	53.7924	1.0525	0.0000	1.0000	-0.0000
X ₃	157.8668	1.4543	0.8580	0.0000	0.5137
V	212.9514	2.7855			

% 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	0.0103	0.0000	0.0007
240.0000	-0.0146	0.8048	2.2498	-0.0343	0.7531	2.2108
250.0000	-0.0190	0.8345	2.4095	-0.0375	0.8069	2.3687
260.0000	-0.0290	0.8499	2.5543	-0.0407	0.8607	2.5265
270.0000	-0.0530	0.9188	2.6770	-0.0438	0.9145	2.6844
280.0000	-0.0479	0.9390	2.8231	-0.0470	0.9683	2.8423
290.0000	-0.0442	0.9805	2.9353	-0.0502	1.0221	3.0001
300.0000	-0.0839	1.0387	3.1149	-0.0534	1.0759	3.1580
310.0000	-0.0779	1.0909	3.2777	-0.0566	1.1296	3.3159
320.0000	-0.0708	1.1859	3.4338	-0.0597	1.1834	3.4737
330.0000	-0.0427	1.2345	3.6068	-0.0629	1.2372	3.6316
340.0000	-0.0414	1.3022	3.8395	-0.0661	1.2910	3.7895
350.0000	-0.0868	1.4078	4.0279	-0.0693	1.3448	3.9473

Volume

T	V (Å ³)	V _{lin} (Å ³)
100.0000	1310.3650	1310.1233
240.0000	1350.5946	1349.1895
250.0000	1353.0650	1351.9799
260.0000	1355.0731	1354.7704
270.0000	1357.3213	1357.5608
280.0000	1359.6183	1360.3513
290.0000	1361.7309	1363.1417
300.0000	1364.3892	1365.9321
310.0000	1367.3633	1368.7226
320.0000	1370.8472	1371.5130
330.0000	1374.2223	1374.3035
340.0000	1378.3002	1377.0939
350.0000	1381.6758	1379.8843

Input

T	σ T	a	b	c	α	β	γ
350	2	8.501	8.5428	19.105	90	95.229	90
340	2	8.4971	8.5339	19.091	90	95.360	90
330	2	8.4909	8.5282	19.065	90	95.482	90
320	2	8.4829	8.5241	19.048	90	95.567	90
310	2	8.4772	8.5161	19.033	90	95.652	90
300	2	8.4728	8.5117	19.014	90	95.734	90
290	2	8.4738	8.5068	18.989	90	95.834	90
280	2	8.4708	8.5033	18.976	90	95.891	90
270	2	8.4669	8.5016	18.959	90	95.965	90
260	2	8.4648	8.4958	18.948	90	96.045	90
250	2	8.4628	8.4945	18.930	90	96.122	90
240	2	8.4610	8.4920	18.9078	90	96.200	90
100	2	8.4066	8.4242	18.659	90	97.413	90