

Output

Axes			Direction		
	$\alpha(\text{MK}^{-1})$	$\sigma\alpha(\text{MK}^{-1})$	a	b	c
X_1	25.5097	1.8511	0.6670	-0.0000	-0.7450
X_2	67.2175	1.9976	0.0000	-1.0000	0.0000
X_3	83.6854	3.5167	0.9719	-0.0000	0.2352
V	180.6450	5.9503			

% change in length

T	X_1	X_2	X_3	$X_{1,\text{calc}}$	$X_{2,\text{calc}}$	$X_{3,\text{calc}}$
100.0000	0.0000	0.0000	0.0000	-0.0382	-0.0642	-0.0774
110.0000	0.0069	0.0612	0.0657	-0.0127	0.0030	0.0063
120.0000	0.0205	0.0836	0.1260	0.0128	0.0703	0.0900
130.0000	0.0313	0.0907	0.1402	0.0384	0.1375	0.1737
140.0000	0.0589	0.2131	0.2934	0.0639	0.2047	0.2574
150.0000	0.0626	0.2096	0.2831	0.0894	0.2719	0.3411
160.0000	0.0981	0.2885	0.3633	0.1149	0.3391	0.4247
170.0000	0.1398	0.3674	0.4999	0.1404	0.4063	0.5084
180.0000	0.1452	0.4781	0.5604	0.1659	0.4736	0.5921
190.0000	0.1497	0.5098	0.6125	0.1914	0.5408	0.6758
200.0000	0.2213	0.6347	0.7444	0.2169	0.6080	0.7595
210.0000	0.2209	0.6582	0.7779	0.2424	0.6752	0.8432
220.0000	0.2461	0.7242	0.8573	0.2679	0.7424	0.9269
230.0000	0.3066	0.8266	1.0127	0.2935	0.8096	1.0105
240.0000	0.3903	0.9196	1.1174	0.3190	0.8769	1.0942
250.0000	0.3953	0.9491	1.2161	0.3445	0.9441	1.1779
260.0000	0.3268	1.0362	1.3957	0.3700	1.0113	1.2616

Volume

T	V (\AA^3)	V _{lin} (\AA^3)
100.0000	1299.7134	1297.0320
110.0000	1301.4535	1299.3799
120.0000	1302.7071	1301.7277
130.0000	1303.1237	1304.0756
140.0000	1307.0751	1306.4235
150.0000	1306.9430	1308.7713
160.0000	1309.4824	1311.1192
170.0000	1312.8447	1313.4671
180.0000	1315.1553	1315.8150
190.0000	1316.3125	1318.1628
200.0000	1320.6187	1320.5107
210.0000	1321.3641	1322.8586
220.0000	1323.6028	1325.2064
230.0000	1327.7943	1327.5543
240.0000	1331.5098	1329.9022
250.0000	1333.2678	1332.2500
260.0000	1335.8858	1334.5979

Input

T	σT	a	b	c	α	β	γ
260	2	8.5191	8.5807	18.450	90	97.902	90
250	2	8.5136	8.5733	18.448	90	98.043	90
240	2	8.5071	8.5708	18.445	90	98.084	90
230	2	8.5015	8.5629	18.424	90	98.114	90
220	2	8.4918	8.5542	18.408	90	98.168	90
210	2	8.4857	8.5486	18.403	90	98.187	90
200	2	8.4837	8.5466	18.402	90	98.203	90
190	2	8.4752	8.5360	18.385	90	98.242	90
180	2	8.4718	8.5333	18.383	90	98.263	90
170	2	8.4665	8.5239	18.383	90	98.275	90
160	2	8.4581	8.5172	18.371	90	98.327	90

150	2	8.4525	8.5105	18.363	90	98.349	90
140	2	8.4512	8.5108	18.366	90	98.327	90
130	2	8.4431	8.5004	18.354	90	98.402	90
120	2	8.4403	8.4998	18.3549	90	98.389	90
110	2	8.4372	8.4979	18.3494	90	98.417	90
100	2	8.4330	8.4927	18.3465	90	98.444	90