

Output

Axes			Direction		
	α (MK ⁻¹)	$\sigma\alpha$ (MK ⁻¹)	a	b	c
X ₁	-5.9941	0.5811	-0.9511	0.0000	0.3088
X ₂	44.3186	0.4844	0.0000	1.0000	-0.0000
X ₃	167.0034	0.2018	0.8660	-0.0000	0.5001
V	208.5841	0.4348			

% 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	0.0060	-0.0000	0.0004
270.0000	-0.1013	0.7563	2.8463	-0.0959	0.7534	2.8395
280.0000	-0.1075	0.8037	3.0139	-0.1019	0.7977	3.0065
290.0000	-0.1059	0.8629	3.1698	-0.1079	0.8420	3.1735
300.0000	-0.0957	0.8867	3.3301	-0.1139	0.8863	3.3405
310.0000	-0.1029	0.9080	3.5136	-0.1199	0.9306	3.5075
320.0000	-0.1007	0.9471	3.6608	-0.1259	0.9750	3.6745
330.0000	-0.1381	0.9957	3.8402	-0.1319	1.0193	3.8415
340.0000	-0.1409	1.0917	4.0051	-0.1379	1.0636	4.0085
350.0000	-0.1802	1.1237	4.1880	-0.1439	1.1079	4.1755

Volume

T	V (Å ³)	V _{lin} (Å ³)
100.0000	1318.1248	1318.1132
270.0000	1364.7922	1364.8530
280.0000	1367.6083	1367.6024
290.0000	1370.5354	1370.3518
300.0000	1373.1579	1373.1012
310.0000	1375.8303	1375.8506
320.0000	1378.3855	1378.6000
330.0000	1380.9727	1381.3494
340.0000	1384.4856	1384.0988
350.0000	1386.8759	1386.8482

Input

T	σ T	a	b	c	α	β	γ
350	2	8.5199	8.5310	19.1569	90	95.099	90
340	2	8.5152	8.5283	19.1443	90	95.225	90
330	2	8.5108	8.5202	19.1265	90	95.314	90
320	2	8.5082	8.5161	19.1093	90	95.429	90
310	2	8.5031	8.5128	19.0953	90	95.510	90
300	2	8.4989	8.5110	19.0749	90	95.610	90
290	2	8.4944	8.5090	19.0556	90	95.688	90
280	2	8.4921	8.5040	19.0337	90	95.762	90
270	2	8.4884	8.5000	19.0148	90	95.853	90
100	2	8.4204	8.4362	18.7134	90	97.444	90