Output

			Direction		
Axes	α(MK^{-1})	σα (MK^{-1})	a	b	c
X_1	18.9351	1.9155	0.4728	0.8811	-0.0000
X_2	18.7205	1.9399	-0.9987	0.0500	0.0000
X_3	75.2305	5.5502	0.0000	0.0000	1.0000
V	119.3715	8.9525			

% change in length

T	X_1	X_2	X_3	$X_{1,calc}$	$X_{2,calc}$	$X_{3,calc}$
10.0000	0.0000	0.0000	0.0000	-0.0160	-0.0146	-0.0778
15.0000	0.0063	0.0093	0.0093	-0.0065	-0.0052	-0.0402
20.0000	0.0063	0.0093	0.0093	0.0029	0.0042	-0.0026
30.0000	0.0187	0.0187	0.0376	0.0219	0.0229	0.0727
40.0000	0.0280	0.0280	0.0878	0.0408	0.0416	0.1479
50.0000	0.0467	0.0467	0.1567	0.0597	0.0603	0.2231
60.0000	0.0654	0.0654	0.2445	0.0787	0.0790	0.2984
70.0000	0.0841	0.0841	0.3354	0.0976	0.0978	0.3736
80.0000	0.1028	0.1028	0.4545	0.1165	0.1165	0.4488
90.0000	0.1402	0.1402	0.5643	0.1355	0.1352	0.5241
100.0000	0.1869	0.1869	0.6677	0.1544	0.1539	0.5993

Volume

T	V (Å^3)	V_{lin} (Å^3)
10.0000	3163.5161	3159.2588
15.0000	3164.3057	3161.1470
20.0000	3164.3057	3163.0351
30.0000	3165.8892	3166.8115
40.0000	3168.0684	3170.5878
50.0000	3171.4362	3174.3641
60.0000	3175.4016	3178.1405
70.0000	3179.4686	3181.9168
80.0000	3184.4324	3185.6931
90.0000	3190.2918	3189.4695
100.0000	3196.5544	3193.2458

Input

T	σT	a	b	c	α	β	γ
10	2	10.701	10.701	31.9	90	90	120
15	2	10.702	10.702	31.902	90	90	120
20	2	10.702	10.702	31.902	90	90	120
30	2	10.703	10.703	31.912	90	90	120
40	2	10.704	10.704	31.928	90	90	120
50	2	10.706	10.706	31.95	90	90	120
60	2	10.708	10.708	31.978	90	90	120
70	2	10.71	10.71	32.007	90	90	120
80	2	10.712	10.712	32.045	90	90	120
90	2	10.716	10.716	32.08	90	90	120
100	2	10.721	10.721	32.113	90	90	120