Output

			Direction		
Axes	$\alpha(MK^{-1})$	$\sigma\alpha\ (MK^{-1})$	a	b	c
X_1	-17.6446	2.1067	-0.0416	-0.0000	0.9991
X_2	78.0440	2.7813	0.0000	1.0000	0.0000
X_3	179.6673	1.8712	-0.9220	0.0000	-0.3873
V	242.0090	1.7703			

% change in length

T	X_1	X_2	X_3	$X_{1,calc}$	$X_{2,calc}$	$X_{3,calc}$
90.0000	0.0000	0.0000	0.0000	0.0005	0.0272	-0.0398
100.0000	0.0159	0.0493	0.1372	-0.0172	0.1052	0.1399
125.0000	-0.0392	0.3152	0.5283	-0.0613	0.3003	0.5890
150.0000	-0.1082	0.5122	1.0139	-0.1054	0.4955	1.0382
175.0000	-0.1737	0.7289	1.4946	-0.1495	0.6906	1.4874
200.0000	-0.2597	0.9555	1.9789	-0.1936	0.8857	1.9365
250.0000	-0.2996	1.2904	2.8678	-0.2818	1.2759	2.8349
290.0000	-0.2962	1.5169	3.5189	-0.3524	1.5881	3.5535

Volume

T	V ($Å^3$)	V_{lin} ($Å^3$)
90.0000	3043.7435	3043.2153
100.0000	3049.9069	3050.5815
125.0000	3068.2662	3068.9968
150.0000	3087.0092	3087.4122
175.0000	3106.3496	3105.8275
200.0000	3125.4972	3124.2428
250.0000	3161.9371	3161.0735
290.0000	3189.1780	3190.5380

Input

T	σT	a	b	c	α	β	γ
290	2	18.128	10.306	18.598	90	113.386	90
250	2	18.037	10.283	18.597	90	113.552	90
200	2	17.914	10.249	18.604	90	113.789	90
175	2	17.847	10.226	18.62	90	113.92	90
150	2	17.782	10.204	18.632	90	114.06	90
125	2	17.713	10.184	18.645	90	114.18	90
100	2	17.661	10.157	18.655	90	114.3	90
90	2	17.641	10.152	18.652	90	114.33	90