

Output

Axes			Direction		
	$\alpha$ (MK <sup>-1</sup> )	$\sigma\alpha$ (MK <sup>-1</sup> )	a	b	c
X <sub>1</sub>	5.4416	0.2775	-0.9474	0.0000	0.3200
X <sub>2</sub>	59.0210	0.4361	0.0000	1.0000	-0.0000
X <sub>3</sub>	182.2314	0.5060	0.8698	-0.0000	0.4934
V	251.4922	1.1772			

% change in length

T	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>1,calc</sub>	X <sub>2,calc</sub>	X <sub>3,calc</sub>
100.0000	0.0000	0.0000	0.0000	0.0034	-0.0000	-0.0001
290.0000	0.1172	1.1382	3.4473	0.1068	1.1214	3.4623
300.0000	0.1116	1.1760	3.6596	0.1122	1.1804	3.6445
310.0000	0.1377	1.2539	3.8387	0.1177	1.2394	3.8267
320.0000	0.1155	1.2575	3.9990	0.1231	1.2984	4.0090
330.0000	0.1224	1.3555	4.2077	0.1286	1.3575	4.1912
340.0000	0.1153	1.4062	4.3348	0.1340	1.4165	4.3734
350.0000	0.1457	1.5019	4.5757	0.1394	1.4755	4.5557

Volume

T	V (Å <sup>3</sup> )	V <sub>lin</sub> (Å <sup>3</sup> )
100.0000	1305.8306	1305.7747
290.0000	1368.1822	1368.1719
300.0000	1371.4726	1371.4559
310.0000	1375.2928	1374.7400
320.0000	1377.2032	1378.0241
330.0000	1381.4491	1381.3081
340.0000	1383.7649	1384.5922
350.0000	1388.7479	1387.8763

Input

T	$\sigma T$	a	b	c	$\alpha$	$\beta$	$\gamma$
350	2	8.5444	8.5967	19.0030	90	95.778	90
340	2	8.5359	8.5886	18.9753	90	95.889	90
330	2	8.5310	8.5843	18.9666	90	95.967	90
320	2	8.5251	8.5760	18.9434	90	96.073	90
310	2	8.5223	8.5757	18.9274	90	96.169	90
300	2	8.5172	8.5691	18.9034	90	96.245	90
290	2	8.5123	8.5659	18.8801	90	96.359	90
100	2	8.4150	8.4695	18.5093	90	98.156	90