

Output

Axes	Direction				
	α (MK ⁻¹)	$\sigma\alpha$ (MK ⁻¹)	a	b	c
X ₁	-26.2591	3.3365	0.0046	-0.0000	1.0000
X ₂	68.5291	0.8768	0.0000	-1.0000	0.0000
X ₃	183.8558	2.3722	0.9332	0.0000	0.3594
V	227.3039	1.4043			

% 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	-0.0741	0.0235	-0.0030
100.0000	-0.0394	0.0729	0.1441	-0.1003	0.0920	0.1809
125.0000	-0.1532	0.2649	0.5874	-0.1660	0.2634	0.6405
150.0000	-0.2762	0.4550	1.0914	-0.2316	0.4347	1.1002
175.0000	-0.3822	0.6322	1.6019	-0.2973	0.6060	1.5598
200.0000	-0.4533	0.7898	2.0896	-0.3629	0.7773	2.0194
220.0000	-0.4849	0.9375	2.4522	-0.4155	0.9144	2.3871
250.0000	-0.5036	1.1147	2.9665	-0.4942	1.1200	2.9387
270.0000	-0.5030	1.2428	3.2842	-0.5467	1.2570	3.3064
290.0000	-0.4921	1.3727	3.5868	-0.5993	1.3941	3.6741

Volume

T	V (Å ³)	V _{lin} (Å ³)
90.0000	3043.4068	3041.6338
100.0000	3048.8103	3048.5516
125.0000	3064.6907	3065.8461
150.0000	3082.0841	3083.1405
175.0000	3099.8153	3100.4350
200.0000	3117.3456	3117.7295
220.0000	3132.0072	3131.5650
250.0000	3152.6657	3152.3184
270.0000	3166.4180	3166.1539
290.0000	3180.1195	3179.9895

Input

T	σ T	a	b	c	α	β	γ
290	2	18.1511	10.2942	18.5301	90	113.295	90
270	2	18.1081	10.281	18.528	90	113.368	90
250	2	18.0638	10.268	18.5278	90	113.451	90
220	2	17.9925	10.25	18.5312	90	113.589	90
200	2	17.9421	10.235	18.5371	90	113.686	90
175	2	17.8743	10.219	18.5504	90	113.817	90
150	2	17.803	10.201	18.5702	90	113.952	90
125	2	17.7314	10.1817	18.5931	90	114.0765	90
100	2	17.6675	10.1622	18.6142	90	114.1791	90
90	2	17.6467	10.1548	18.6215	90	114.2122	90