

Output

		Direction			
Axes	α (MK ⁻¹)	$\sigma\alpha$ (MK ⁻¹)	a	b	c
X ₁	-49.9855	3.4308	0.2318	0.9728	-0.0000
X ₂	-49.9855	3.4308	0.9586	0.2848	-0.0000
X ₃	380.7929	12.6577	-0.0000	-0.0000	1.0000
V	277.0111	6.6463			

% change in length

T	X ₁	X ₂	X ₃	X _{1,calc}	X _{2,calc}	X _{3,calc}
140.0000	0.0000	0.0000	0.0000	0.1183	0.1183	-0.3806
150.0000	0.0175	0.0175	0.1781	0.0683	0.0683	0.0002
160.0000	0.0230	0.0230	0.3874	0.0183	0.0183	0.3810
180.0000	-0.0009	-0.0009	0.9092	-0.0816	-0.0816	1.1426
200.0000	-0.0782	-0.0782	1.5810	-0.1816	-0.1816	1.9042
220.0000	-0.1996	-0.1996	2.3903	-0.2816	-0.2816	2.6658
240.0000	-0.3606	-0.3606	3.3026	-0.3815	-0.3815	3.4274
260.0000	-0.5050	-0.5050	4.1900	-0.4815	-0.4815	4.1889
280.0000	-0.6173	-0.6173	4.9992	-0.5815	-0.5815	4.9505
290.0000	-0.6596	-0.6596	5.3679	-0.6315	-0.6315	5.3313
300.0000	-0.7166	-0.7166	6.0178	-0.6815	-0.6815	5.7121

Volume

T	V (Å ³)	V _{lin} (Å ³)
140.0000	3275.3333	3270.7885
150.0000	3282.3136	3279.8615
160.0000	3289.5357	3288.9346
180.0000	3305.0529	3307.0807
200.0000	3321.9153	3325.2267
220.0000	3340.2463	3343.3728
240.0000	3359.1465	3361.5189
260.0000	3378.1867	3379.6649
280.0000	3396.7492	3397.8110
290.0000	3405.7744	3406.8841
300.0000	3422.8471	3415.9571

Input

T	σ T	a	b	c	α	β	γ
140	2	10.8706	10.8706	32.005	90	90	120
150	2	10.8725	10.8725	32.062	90	90	120
160	2	10.8731	10.8731	32.129	90	90	120
180	2	10.8705	10.8705	32.296	90	90	120
200	2	10.8621	10.8621	32.511	90	90	120
220	2	10.8489	10.8489	32.77	90	90	120
240	2	10.8314	10.8314	33.062	90	90	120
260	2	10.8157	10.8157	33.346	90	90	120
280	2	10.8035	10.8035	33.605	90	90	120
290	2	10.7989	10.7989	33.723	90	90	120
300	2	10.7927	10.7927	33.931	90	90	120