

Output

Axes			Direction		
	α (MK ⁻¹)	$\sigma\alpha$ (MK ⁻¹)	a	b	c
X ₁	8.2745	2.1126	0.9503	-0.0000	-0.3113
X ₂	48.9362	2.0159	0.0000	-1.0000	0.0000
X ₃	80.4520	4.1889	0.8631	-0.0000	0.5051
V	140.4108	6.5183			

% change in length

T	X ₁	X ₂	X ₃	X _{1,calc}	X _{2,calc}	X _{3,calc}
100.0000	0.0000	0.0000	0.0000	-0.0275	-0.0034	-0.0417
110.0000	-0.0342	0.0531	0.0542	-0.0192	0.0455	0.0388
120.0000	-0.0258	0.0700	0.0885	-0.0109	0.0944	0.1192
130.0000	-0.0038	0.1558	0.1783	-0.0026	0.1434	0.1997
150.0000	0.0063	0.2349	0.3149	0.0139	0.2412	0.3606
160.0000	0.0221	0.2880	0.4191	0.0222	0.2902	0.4410
170.0000	0.0344	0.3659	0.5513	0.0305	0.3391	0.5215
180.0000	0.0462	0.3707	0.6345	0.0387	0.3880	0.6019

Volume

T	V (Å ³)	V _{lin} (Å ³)
100.0000	1313.8869	1312.8048
110.0000	1314.8472	1314.6496
120.0000	1315.6313	1316.4945
130.0000	1318.2318	1318.3393
150.0000	1321.2070	1322.0290
160.0000	1323.4917	1323.8738
170.0000	1326.4289	1325.7187
180.0000	1327.7484	1327.5635

Input

T	σ T	a	b	c	α	β	γ
180	2	8.4554	8.5030	18.6152	90	97.2210	90
170	2	8.4532	8.5026	18.6039	90	97.2570	90
160	2	8.4487	8.4960	18.5898	90	97.324	90
150	2	8.4458	8.4915	18.5758	90	97.3690	90
130	2	8.4415	8.4848	18.5610	90	97.4390	90
120	2	8.4373	8.4791	18.5481	90	97.4870	90
110	2	8.4350	8.4761	18.5496	90	97.5090	90
100	2	8.4375	8.4716	18.5416	90	97.5370	90