

Output

Axes			Direction		
	$\alpha(\text{MK}^{-1})$	$\sigma\alpha(\text{MK}^{-1})$	a	b	c
X_1	-71.8486	3.2857	0.0000	-1.0000	0.0000
X_2	31.9327	0.7909	0.9716	-0.0000	0.2366
X_3	180.1341	2.9361	-0.0091	-0.0000	1.0000
V	139.8849	1.9469			

% change in length

T	X_1	X_2	X_3	$X_{1,\text{calc}}$	$X_{2,\text{calc}}$	$X_{3,\text{calc}}$
120.0000	0.0000	0.0000	0.0000	-0.0163	-0.0023	0.0095
130.0000	-0.0994	0.0268	0.1918	-0.0881	0.0296	0.1897
140.0000	-0.1663	0.0613	0.3765	-0.1600	0.0615	0.3698
150.0000	-0.2445	0.0948	0.5598	-0.2318	0.0935	0.5499
160.0000	-0.3016	0.1213	0.7379	-0.3037	0.1254	0.7301
165.0000	-0.3277	0.1449	0.8031	-0.3396	0.1414	0.8201

Volume

T	V (\AA^3)	V _{lin} (\AA^3)
120.0000	3731.6870	3731.3441
130.0000	3736.1258	3736.5642
140.0000	3741.8001	3741.7843
150.0000	3746.9494	3747.0043
160.0000	3752.4314	3752.2244
165.0000	3754.7621	3754.8344

Input

T	σT	a	b	c	α	β	γ
120	2	19.6218	12.2678	15.7743	90	100.653	90
130	2	19.6277	12.2556	15.8045	90	100.662	90
140	2	19.6351	12.2474	15.8336	90	100.671	90
150	2	19.6439	12.2378	15.8626	90	100.707	90
160	2	19.65	12.2308	15.8907	90	100.721	90
165	2	19.6561	12.2276	15.9009	90	100.742	90