

Output

| | | | Direction | | |
|----------------------|--------------------------|--------------------------------|-----------|---------|---------|
| Axes | $\alpha(\text{MK}^{-1})$ | $\sigma\alpha(\text{MK}^{-1})$ | a | b | c |
| X₁ | 25.3318 | 0.6173 | 0.9193 | -0.0000 | -0.3936 |
| X₂ | 57.8174 | 0.7583 | 0.0000 | -1.0000 | 0.0000 |
| X₃ | 93.4890 | 2.7236 | 0.9003 | -0.0000 | 0.4354 |
| V | 180.3806 | 4.1898 | | | |

% 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 | -0.0486 | -0.0258 | -0.1386 |
| 110.0000 | -0.0232 | 0.0506 | 0.0665 | -0.0232 | 0.0320 | -0.0451 |
| 120.0000 | 0.0043 | 0.0930 | 0.1214 | 0.0021 | 0.0898 | 0.0484 |
| 130.0000 | 0.0615 | 0.1365 | 0.2429 | 0.0274 | 0.1477 | 0.1419 |
| 140.0000 | 0.0466 | 0.2036 | 0.2583 | 0.0528 | 0.2055 | 0.2354 |
| 150.0000 | 0.0581 | 0.2718 | 0.3239 | 0.0781 | 0.2633 | 0.3288 |
| 160.0000 | 0.0640 | 0.2977 | 0.3782 | 0.1034 | 0.3211 | 0.4223 |
| 170.0000 | 0.1090 | 0.3742 | 0.4677 | 0.1288 | 0.3789 | 0.5158 |
| 180.0000 | 0.1341 | 0.4259 | 0.5516 | 0.1541 | 0.4367 | 0.6093 |
| 190.0000 | 0.1523 | 0.4965 | 0.6173 | 0.1794 | 0.4946 | 0.7028 |
| 200.0000 | 0.2361 | 0.5483 | 0.7540 | 0.2048 | 0.5524 | 0.7963 |
| 210.0000 | 0.2245 | 0.6013 | 0.8185 | 0.2301 | 0.6102 | 0.8898 |
| 220.0000 | 0.2700 | 0.6954 | 0.9207 | 0.2554 | 0.6680 | 0.9833 |
| 230.0000 | 0.2790 | 0.7530 | 1.0053 | 0.2807 | 0.7258 | 1.0768 |
| 240.0000 | 0.3050 | 0.7942 | 1.0800 | 0.3061 | 0.7836 | 1.1702 |
| 250.0000 | 0.3160 | 0.8272 | 1.1815 | 0.3314 | 0.8415 | 1.2637 |
| 260.0000 | 0.3650 | 0.8836 | 1.2995 | 0.3567 | 0.8993 | 1.3572 |
| 270.0000 | 0.3705 | 0.9295 | 1.3867 | 0.3821 | 0.9571 | 1.4507 |
| 280.0000 | 0.4232 | 0.9978 | 1.5043 | 0.4074 | 1.0149 | 1.5442 |
| 290.0000 | 0.4244 | 1.0366 | 1.5941 | 0.4327 | 1.0727 | 1.6377 |
| 300.0000 | 0.4683 | 1.1190 | 1.7298 | 0.4581 | 1.1306 | 1.7312 |
| 310.0000 | 0.4645 | 1.1766 | 1.8089 | 0.4834 | 1.1884 | 1.8247 |
| 320.0000 | 0.4987 | 1.2343 | 1.9521 | 0.5087 | 1.2462 | 1.9182 |
| 330.0000 | 0.5306 | 1.2955 | 2.0781 | 0.5341 | 1.3040 | 2.0116 |
| 340.0000 | 0.5741 | 1.3849 | 2.2506 | 0.5594 | 1.3618 | 2.1051 |
| 350.0000 | 0.6134 | 1.4931 | 2.3881 | 0.5847 | 1.4196 | 2.1986 |

Volume

| T | V (Å ³) | V _{lin} (Å ³) |
|----------|---------------------|------------------------------------|
| 100.0000 | 1306.6181 | 1303.4752 |
| 110.0000 | 1307.8454 | 1305.8320 |
| 120.0000 | 1309.4778 | 1308.1889 |
| 130.0000 | 1312.3881 | 1310.5458 |
| 140.0000 | 1313.2723 | 1312.9027 |
| 150.0000 | 1315.1797 | 1315.2596 |
| 160.0000 | 1316.3097 | 1317.6165 |
| 170.0000 | 1319.0824 | 1319.9734 |
| 180.0000 | 1321.1957 | 1322.3302 |
| 190.0000 | 1323.2316 | 1324.6871 |
| 200.0000 | 1326.8220 | 1327.0440 |
| 210.0000 | 1328.2208 | 1329.4009 |
| 220.0000 | 1331.4162 | 1331.7578 |
| 230.0000 | 1333.4186 | 1334.1147 |
| 240.0000 | 1335.2994 | 1336.4716 |
| 250.0000 | 1337.2286 | 1338.8284 |
| 260.0000 | 1340.1959 | 1341.1853 |
| 270.0000 | 1342.0388 | 1343.5422 |
| 280.0000 | 1345.2144 | 1345.8991 |
| 290.0000 | 1346.9442 | 1348.2560 |
| 300.0000 | 1350.4401 | 1350.6129 |
| 310.0000 | 1352.2161 | 1352.9698 |
| 320.0000 | 1355.3610 | 1355.3266 |

330.0000 1358.2977 1357.6835
340.0000 1362.3969 1360.0404
350.0000 1366.2306 1362.3973

Input

| | T | σT | a | b | c | α | β | γ |
|-----|---|------------|--------|---------|----|----------|---------|----------|
| 350 | 2 | 8.5450 | 8.6258 | 18.6681 | 90 | 96.824 | 90 | |
| 340 | 2 | 8.5366 | 8.6166 | 18.6562 | 90 | 96.882 | 90 | |
| 330 | 2 | 8.5292 | 8.6090 | 18.6354 | 90 | 96.952 | 90 | |
| 320 | 2 | 8.5248 | 8.6038 | 18.6179 | 90 | 97.001 | 90 | |
| 310 | 2 | 8.5190 | 8.5989 | 18.6003 | 90 | 97.060 | 90 | |
| 300 | 2 | 8.5157 | 8.5940 | 18.5956 | 90 | 97.108 | 90 | |
| 290 | 2 | 8.5085 | 8.5870 | 18.5804 | 90 | 97.160 | 90 | |
| 280 | 2 | 8.5053 | 8.5837 | 18.5727 | 90 | 97.210 | 90 | |
| 270 | 2 | 8.5000 | 8.5779 | 18.5543 | 90 | 97.243 | 90 | |
| 260 | 2 | 8.4976 | 8.5740 | 18.5443 | 90 | 97.287 | 90 | |
| 250 | 2 | 8.4914 | 8.5692 | 18.5287 | 90 | 97.325 | 90 | |
| 240 | 2 | 8.4884 | 8.5664 | 18.5166 | 90 | 97.374 | 90 | |
| 230 | 2 | 8.4863 | 8.5629 | 18.5037 | 90 | 97.399 | 90 | |
| 220 | 2 | 8.4824 | 8.5580 | 18.4968 | 90 | 97.442 | 90 | |
| 210 | 2 | 8.4752 | 8.5500 | 18.4868 | 90 | 97.476 | 90 | |
| 200 | 2 | 8.4728 | 8.5455 | 18.4842 | 90 | 97.521 | 90 | |
| 190 | 2 | 8.4683 | 8.5411 | 18.4545 | 90 | 97.545 | 90 | |
| 180 | 2 | 8.4639 | 8.5351 | 18.4498 | 90 | 97.572 | 90 | |
| 170 | 2 | 8.4600 | 8.5307 | 18.4397 | 90 | 97.605 | 90 | |
| 160 | 2 | 8.4552 | 8.5242 | 18.4265 | 90 | 97.630 | 90 | |
| 150 | 2 | 8.4548 | 8.5220 | 18.4176 | 90 | 97.660 | 90 | |
| 140 | 2 | 8.4499 | 8.5162 | 18.4153 | 90 | 97.688 | 90 | |
| 130 | 2 | 8.4465 | 8.5105 | 18.4239 | 90 | 97.717 | 90 | |
| 120 | 2 | 8.4433 | 8.5068 | 18.3991 | 90 | 97.742 | 90 | |
| 110 | 2 | 8.4409 | 8.5032 | 18.3900 | 90 | 97.761 | 90 | |
| 100 | 2 | 8.4381 | 8.4989 | 18.3902 | 90 | 97.808 | 90 | |