

Output

3 data points entered - at least as many data points as parameters are needed for a fit to be carried out (i.e. 3 for 3rd order Birch-Murnaghan,4 for empirical pressure fitting). As PASCAL calculates errors from derivatives, more data points than parameters are needed for error estimates.

| Direction | | | | | |
|-----------|--------------------------|--------------------------------|---------|---------|---------|
| Axes | $\alpha(\text{MK}^{-1})$ | $\sigma\alpha(\text{MK}^{-1})$ | a | b | c |
| X_1 | 66.1008 | 0.6378 | 0.0000 | -1.0000 | 0.0000 |
| X_2 | 71.3313 | 1.5117 | -0.2625 | 0.0000 | -0.9649 |
| X_3 | 146.2573 | 2.5830 | 0.9937 | -0.0000 | -0.1122 |
| V | 285.1436 | 4.6386 | | | |

% change in length

| T | X_1 | X_2 | X_3 | $X_{1,\text{calc}}$ | $X_{2,\text{calc}}$ | $X_{3,\text{calc}}$ |
|----------|--------|--------|--------|---------------------|---------------------|---------------------|
| 290.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0018 | 0.0043 | 0.0073 |
| 310.0000 | 0.1376 | 0.1555 | 0.3144 | 0.1340 | 0.1469 | 0.2998 |
| 330.0000 | 0.2644 | 0.2853 | 0.5850 | 0.2662 | 0.2896 | 0.5923 |

Volume

| T | V (\AA^3) | V _{lin} (\AA^3) |
|----------|----------------------|-------------------------------------|
| 290.0000 | 3118.2037 | 3118.5839 |
| 310.0000 | 3137.1836 | 3136.3667 |
| 330.0000 | 3153.7127 | 3154.1494 |

Input

| T | σT | a | b | c | α | β | γ |
|-----|------------|---------|---------|---------|----------|---------|----------|
| 290 | 2 | 10.5677 | 19.4022 | 15.2137 | 90 | 91.564 | 90 |
| 310 | 2 | 10.6005 | 19.4289 | 15.2382 | 90 | 91.595 | 90 |
| 330 | 2 | 10.6286 | 19.4535 | 15.2589 | 90 | 91.626 | 90 |