

# Output

4 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           | $\alpha$ (MK <sup>-1</sup> ) | $\sigma\alpha$ (MK <sup>-1</sup> ) | a      | b       | c       |  |
| X <sub>1</sub> | -16.2222                     | 1.2124                             | 0.0180 | 0.0000  | -0.9998 |  |
| X <sub>2</sub> | 14.8721                      | 3.6429                             | 0.0000 | -1.0000 | 0.0000  |  |
| X <sub>3</sub> | 40.3315                      | 6.8613                             | 0.9234 | 0.0000  | 0.3839  |  |
| V              | 53.3555                      | 11.0024                            |        |         |         |  |

## % change in length

| T       | X <sub>1</sub> | X <sub>2</sub> | X <sub>3</sub> | X <sub>1,calc</sub> | X <sub>2,calc</sub> | X <sub>3,calc</sub> |
|---------|----------------|----------------|----------------|---------------------|---------------------|---------------------|
| 20.0000 | 0.0000         | 0.0000         | 0.0000         | -0.0027             | -0.0099             | -0.0161             |
| 30.0000 | -0.0217        | -0.0099        | 0.0067         | -0.0190             | 0.0050              | 0.0243              |
| 40.0000 | -0.0378        | 0.0198         | 0.0516         | -0.0352             | 0.0198              | 0.0646              |
| 50.0000 | -0.0487        | 0.0397         | 0.1195         | -0.0514             | 0.0347              | 0.1049              |

## Volume

| T       | V (Å <sup>3</sup> ) | V <sub>lin</sub> (Å <sup>3</sup> ) |
|---------|---------------------|------------------------------------|
| 20.0000 | 2957.8629           | 2956.3756                          |
| 30.0000 | 2957.1251           | 2957.9538                          |
| 40.0000 | 2958.8550           | 2959.5320                          |
| 50.0000 | 2961.1286           | 2961.1101                          |

# Input

| T  | $\sigma$ T | a      | b      | c      | $\alpha$ | $\beta$ | $\gamma$ |
|----|------------|--------|--------|--------|----------|---------|----------|
| 50 | 2          | 17.52  | 10.09  | 18.508 | 90       | 115.17  | 90       |
| 40 | 2          | 17.511 | 10.088 | 18.51  | 90       | 115.19  | 90       |
| 30 | 2          | 17.505 | 10.085 | 18.513 | 90       | 115.203 | 90       |
| 20 | 2          | 17.505 | 10.086 | 18.517 | 90       | 115.211 | 90       |