

Supplementary information for:

**THERMOELASTIC PROPERTIES OF ZIRCON: IMPLICATIONS FOR
GEOTHERMOBAROMETRY**

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Data in Table 3 of the main paper are the results of fitting elastic constants using the software program rpr. Set out below are the output files for each fit, with the format as described in Migliori and Sarrao (1997). Zero values in the second column labells ‘fex’ of the main table, ie 0.000000, represent peaks for which it was not possible to determine resonance frequencies in the primary RUS spectra. Experimental uncertainties quoted in Table 3 were taken from the final matrix of each output file.

Migliori, A., and Sarrao, J.L., Eds. (1997) Resonant ultrasound spectroscopy: applications to physics, material measurements and non-destructive evaluation, 201 p., Wiley, New York.

zircon 293 K cool
 free moduli are c11, c33, c23, c12, c44, c66
 using 12 order polynomials mass= 0.3167 gm rho= 4.661 gm/cc

| n | fex | fr | %err | wt | k | i | df/d(moduli) |
|----|----------|----------|-------|------|---|---|-------------------------------|
| 1 | 0.307600 | 0.305403 | -0.71 | 1.00 | 4 | 1 | 0.00 0.00 0.00 0.00 0.17 0.83 |
| 2 | 0.443730 | 0.443834 | 0.02 | 1.00 | 3 | 2 | 0.02 0.00-0.01 0.00 0.00 0.98 |
| 3 | 0.601650 | 0.604120 | 0.41 | 1.00 | 7 | 2 | 0.30 0.04-0.07 0.00 0.00 0.74 |
| 4 | 0.607820 | 0.605633 | -0.36 | 1.00 | 1 | 2 | 0.30 0.04-0.07 0.00 0.00 0.74 |
| 5 | 0.684040 | 0.683891 | -0.02 | 1.00 | 6 | 2 | 0.82 0.01-0.02-0.12 0.31 0.00 |
| 6 | 0.699360 | 0.695890 | -0.50 | 1.00 | 4 | 2 | 0.04 0.00 0.00-0.01 0.95 0.01 |
| 7 | 0.706220 | 0.707426 | 0.17 | 1.00 | 6 | 3 | 0.70 0.13-0.26 0.08 0.34 0.00 |
| 8 | 0.763230 | 0.765339 | 0.28 | 1.00 | 8 | 2 | 0.37 0.03-0.06-0.02 0.34 0.33 |
| 9 | 0.773460 | 0.766801 | -0.86 | 1.00 | 2 | 2 | 0.37 0.03-0.06-0.02 0.35 0.33 |
| 10 | 0.821500 | 0.821829 | 0.04 | 1.00 | 2 | 3 | 0.07 0.01-0.01 0.00 0.93 0.01 |
| 11 | 0.822920 | 0.822479 | -0.05 | 1.00 | 8 | 3 | 0.07 0.01-0.01 0.00 0.93 0.01 |
| 12 | 0.929050 | 0.931302 | 0.24 | 1.00 | 3 | 3 | 0.14 0.01-0.03 0.00 0.00 0.87 |
| 13 | 0.943590 | 0.943169 | -0.04 | 1.00 | 5 | 1 | 1.21 0.00 0.00-0.21 0.00 0.00 |
| 14 | 0.946360 | 0.948923 | 0.27 | 1.00 | 5 | 2 | 1.10 0.26-0.35-0.01 0.00 0.00 |
| 15 | 0.947720 | 0.950565 | 0.30 | 1.00 | 8 | 4 | 0.35 0.04-0.08 0.00 0.54 0.14 |
| 16 | 0.950160 | 0.951463 | 0.14 | 1.00 | 2 | 4 | 0.35 0.04-0.08 0.00 0.54 0.14 |
| 17 | 0.961350 | 0.953306 | -0.84 | 1.00 | 5 | 3 | 1.01 0.45-0.60 0.14 0.00 0.00 |
| 18 | 0.999010 | 1.001893 | 0.29 | 1.00 | 7 | 3 | 0.84 0.27-0.31-0.01 0.01 0.19 |
| 19 | 1.000500 | 1.002768 | 0.23 | 1.00 | 4 | 3 | 0.06 0.01-0.01 0.01 0.83 0.10 |
| 20 | 1.004700 | 1.003227 | -0.15 | 1.00 | 1 | 3 | 0.84 0.27-0.31 0.00 0.01 0.19 |
| 21 | 1.047600 | 1.051458 | 0.37 | 1.00 | 3 | 4 | 0.07 0.02-0.02 0.00 0.00 0.93 |
| 22 | 1.059300 | 1.057688 | -0.15 | 1.00 | 6 | 4 | 0.43 0.05-0.09 0.00 0.34 0.27 |
| 23 | 1.149800 | 1.149135 | -0.06 | 1.00 | 4 | 4 | 0.09 0.01-0.02-0.01 0.39 0.53 |
| 24 | 0.000000 | 1.183155 | 0.00 | 0.00 | 6 | 5 | 0.75 0.09-0.16-0.02 0.33 0.00 |
| 25 | 1.194300 | 1.198047 | 0.31 | 1.00 | 5 | 4 | 0.59 0.51-0.39 0.03 0.02 0.24 |
| 26 | 1.216100 | 1.215480 | -0.05 | 1.00 | 4 | 5 | 0.04 0.01-0.01 0.00 0.34 0.63 |
| 27 | 1.217600 | 1.219190 | 0.13 | 1.00 | 3 | 5 | 0.17 0.78-0.32 0.03 0.25 0.09 |
| 28 | 0.000000 | 1.225699 | 0.00 | 0.00 | 7 | 4 | 0.52 0.33-0.18-0.03 0.20 0.17 |
| 29 | 0.000000 | 1.225747 | 0.00 | 0.00 | 1 | 4 | 0.52 0.33-0.18-0.03 0.20 0.17 |
| 30 | 0.000000 | 1.283695 | 0.00 | 0.00 | 7 | 5 | 0.31 0.71-0.33 0.03 0.19 0.08 |
| 31 | 1.287200 | 1.284065 | -0.24 | 1.00 | 1 | 5 | 0.31 0.71-0.33 0.03 0.19 0.08 |
| 32 | 0.000000 | 1.293118 | 0.00 | 0.00 | 7 | 6 | 0.25 0.21-0.05-0.01 0.13 0.48 |
| 33 | 1.297400 | 1.294523 | -0.22 | 1.00 | 1 | 6 | 0.25 0.21-0.05-0.02 0.13 0.48 |
| 34 | 1.301500 | 1.298133 | -0.26 | 1.00 | 6 | 6 | 0.43 0.04-0.02-0.07 0.62 0.00 |
| 35 | 1.304000 | 1.300249 | -0.29 | 1.00 | 5 | 5 | 0.50 0.55-0.12-0.06 0.13 0.00 |
| 36 | 1.312000 | 1.316845 | 0.37 | 1.00 | 6 | 7 | 0.42 0.16-0.22 0.06 0.58 0.00 |
| 37 | 1.335700 | 1.333826 | -0.14 | 1.00 | 3 | 6 | 0.25 0.33-0.17-0.01 0.54 0.05 |
| 38 | 1.354200 | 1.353784 | -0.03 | 1.00 | 2 | 5 | 0.35 0.07-0.06-0.03 0.57 0.11 |
| 39 | 1.355400 | 1.355758 | 0.03 | 1.00 | 8 | 5 | 0.35 0.07-0.06-0.03 0.56 0.11 |
| 40 | 1.368900 | 1.367787 | -0.08 | 1.00 | 5 | 6 | 0.47 0.46-0.20 0.02 0.09 0.15 |
| 41 | 1.383800 | 1.385025 | 0.09 | 1.00 | 8 | 6 | 0.31 0.07-0.08-0.01 0.61 0.09 |
| 42 | 1.387800 | 1.386168 | -0.12 | 1.00 | 2 | 6 | 0.31 0.07-0.08-0.01 0.61 0.09 |
| 43 | 1.388900 | 1.391381 | 0.18 | 1.00 | 5 | 7 | 0.46 0.53-0.26 0.01 0.04 0.21 |
| 44 | 1.406800 | 1.412642 | 0.42 | 1.00 | 2 | 7 | 0.36 0.05-0.09 0.02 0.45 0.21 |
| 45 | 0.000000 | 1.413717 | 0.00 | 0.00 | 8 | 7 | 0.36 0.05-0.09 0.02 0.46 0.20 |
| 46 | 1.413800 | 1.413880 | 0.01 | 1.00 | 7 | 7 | 0.32 0.10-0.08-0.01 0.04 0.63 |
| 47 | 1.414500 | 1.415005 | 0.04 | 1.00 | 1 | 7 | 0.32 0.10-0.08-0.01 0.04 0.63 |
| 48 | 1.460100 | 1.461472 | 0.09 | 1.00 | 4 | 6 | 0.30 0.03-0.01-0.03 0.68 0.03 |
| 49 | 1.479800 | 1.482866 | 0.21 | 1.00 | 4 | 7 | 0.23 0.09-0.09 0.03 0.68 0.07 |
| 50 | 1.480500 | 1.484791 | 0.29 | 1.00 | 7 | 8 | 0.30 0.34-0.19 0.01 0.40 0.14 |
| 51 | 1.486400 | 1.484888 | -0.10 | 1.00 | 1 | 8 | 0.31 0.35-0.20 0.01 0.39 0.14 |
| 52 | 1.495100 | 1.499983 | 0.33 | 1.00 | 1 | 9 | 0.51 0.59-0.29-0.03 0.17 0.05 |

Bulk Modulus= 2.311

| c11 | c22 | c33 | c23 | c13 | c12 | c44 | c55 | c66 |
|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| 4.3088 | 4.3088 | 4.9677 | 1.5497 | 1.5497 | 0.7489 | 1.1321 | 1.1321 | 0.4903 |

| d1 | d2 | d3 |
|---------|---------|---------|
| 0.46370 | 0.46280 | 0.31660 |

loop# 3 rms error= 0.3085 %, changed by -.0000011 %

length of gradient vector= 0.000000 blamb= 0.000657

| eigenvalues | eigenvectors |
|-------------|--------------------------------|
| 0.00237 | 0.39 0.45-0.55 0.57-0.11 0.05 |
| 0.02973 | 0.58-0.75 0.12 0.30-0.04 0.02 |
| 0.13698 | 0.59 0.11-0.29-0.74 0.09-0.05 |
| 0.45743 | 0.41 0.47 0.78 0.09 0.01 0.00 |
| 3.23092 | -0.01-0.01 0.04-0.16-0.97 0.15 |
| 14.35877 | 0.00 0.00 0.01-0.04 0.16 0.99 |

chisquare increased 2% by the following % changes in independent parameters

| | | | | | |
|-------|-------|-------|------|-------|-------|
| 0.77 | 0.98 | 3.19 | 4.56 | -0.06 | -0.04 |
| 0.25 | -0.36 | 0.17 | 1.50 | -0.01 | -0.01 |
| -0.14 | 0.03 | -0.20 | 1.15 | 0.04 | 0.02 |

zircon 428 K cool
 free moduli are c11, c33, c23, c12, c44, c66
 using 12 order polynomials mass= 0.3167 gm rho= 4.654 gm/cc

| n | fex | fr | %err | wt | k | i | df/d(moduli) |
|----|----------|----------|-------|------|---|---|-------------------------------|
| 1 | 0.307180 | 0.304722 | -0.80 | 1.00 | 4 | 1 | 0.00 0.00 0.00 0.00 0.17 0.83 |
| 2 | 0.442710 | 0.442778 | 0.02 | 1.00 | 3 | 2 | 0.02 0.00-0.01 0.00 0.00 0.98 |
| 3 | 0.599450 | 0.601731 | 0.38 | 1.00 | 7 | 2 | 0.30 0.04-0.07 0.00 0.00 0.73 |
| 4 | 0.605680 | 0.603240 | -0.40 | 1.00 | 1 | 2 | 0.30 0.04-0.07 0.00 0.00 0.73 |
| 5 | 0.679410 | 0.680496 | 0.16 | 1.00 | 6 | 2 | 0.82 0.01-0.02-0.12 0.31 0.00 |
| 6 | 0.695730 | 0.693905 | -0.26 | 1.00 | 4 | 2 | 0.05 0.00 0.00-0.01 0.95 0.01 |
| 7 | 0.701690 | 0.702098 | 0.06 | 1.00 | 6 | 3 | 0.71 0.14-0.27 0.08 0.34 0.00 |
| 8 | 0.759570 | 0.762192 | 0.35 | 1.00 | 8 | 2 | 0.38 0.03-0.06-0.02 0.34 0.33 |
| 9 | 0.769740 | 0.763644 | -0.79 | 1.00 | 2 | 2 | 0.38 0.03-0.06-0.02 0.34 0.33 |
| 10 | 0.817290 | 0.819368 | 0.25 | 1.00 | 2 | 3 | 0.07 0.01-0.01 0.00 0.93 0.01 |
| 11 | 0.818700 | 0.820020 | 0.16 | 1.00 | 8 | 3 | 0.07 0.01-0.01 0.00 0.93 0.01 |
| 12 | 0.925990 | 0.928508 | 0.27 | 1.00 | 3 | 3 | 0.14 0.01-0.03 0.00 0.00 0.87 |
| 13 | 0.936290 | 0.937706 | 0.15 | 1.00 | 5 | 1 | 1.20 0.01-0.02-0.20 0.00 0.00 |
| 14 | 0.941810 | 0.940327 | -0.16 | 1.00 | 5 | 2 | 1.10 0.27-0.36 0.00 0.00 0.00 |
| 15 | 0.943930 | 0.942438 | -0.16 | 1.00 | 5 | 3 | 1.02 0.45-0.60 0.13 0.00 0.00 |
| 16 | 0.947800 | 0.946273 | -0.16 | 1.00 | 8 | 4 | 0.35 0.04-0.08 0.00 0.54 0.14 |
| 17 | 0.956010 | 0.947170 | -0.92 | 1.00 | 2 | 4 | 0.35 0.04-0.08 0.00 0.54 0.15 |
| 18 | 0.992320 | 0.994041 | 0.17 | 1.00 | 7 | 3 | 0.83 0.28-0.32 0.00 0.01 0.20 |
| 19 | 0.994380 | 0.995351 | 0.10 | 1.00 | 1 | 3 | 0.84 0.28-0.32 0.00 0.01 0.20 |
| 20 | 0.999250 | 0.999745 | 0.05 | 1.00 | 4 | 3 | 0.07 0.01-0.01 0.01 0.83 0.10 |
| 21 | 1.044900 | 1.048582 | 0.35 | 1.00 | 3 | 4 | 0.07 0.02-0.03 0.00 0.00 0.93 |
| 22 | 1.053900 | 1.052630 | -0.12 | 1.00 | 6 | 4 | 0.43 0.05-0.10 0.01 0.33 0.28 |
| 23 | 1.145400 | 1.145850 | 0.04 | 1.00 | 4 | 4 | 0.09 0.02-0.02-0.01 0.39 0.53 |
| 24 | 1.182200 | 1.175567 | -0.56 | 1.00 | 6 | 5 | 0.75 0.10-0.17-0.02 0.33 0.00 |
| 25 | 1.186900 | 1.188131 | 0.10 | 1.00 | 5 | 4 | 0.59 0.52-0.40 0.04 0.02 0.24 |
| 26 | 1.210200 | 1.210077 | -0.01 | 1.00 | 3 | 5 | 0.17 0.79-0.34 0.03 0.24 0.10 |
| 27 | 1.212100 | 1.212348 | 0.02 | 1.00 | 4 | 5 | 0.04 0.01-0.01 0.00 0.34 0.63 |
| 28 | 0.000000 | 1.218059 | 0.00 | 0.00 | 7 | 4 | 0.52 0.34-0.19-0.03 0.19 0.17 |
| 29 | 0.000000 | 1.218085 | 0.00 | 0.00 | 1 | 4 | 0.53 0.34-0.19-0.03 0.19 0.17 |
| 30 | 0.000000 | 1.273551 | 0.00 | 0.00 | 7 | 5 | 0.32 0.73-0.35 0.03 0.17 0.09 |
| 31 | 1.279200 | 1.273916 | -0.41 | 1.00 | 1 | 5 | 0.32 0.73-0.35 0.03 0.18 0.09 |
| 32 | 0.000000 | 1.287493 | 0.00 | 0.00 | 7 | 6 | 0.25 0.20-0.05-0.02 0.14 0.47 |
| 33 | 1.289900 | 1.288857 | -0.08 | 1.00 | 1 | 6 | 0.25 0.20-0.05-0.02 0.14 0.46 |
| 34 | 0.000000 | 1.291486 | 0.00 | 0.00 | 5 | 5 | 0.50 0.55-0.13-0.06 0.13 0.00 |
| 35 | 1.297900 | 1.292948 | -0.38 | 1.00 | 6 | 6 | 0.43 0.04-0.02-0.07 0.62 0.00 |
| 36 | 1.304500 | 1.308735 | 0.32 | 1.00 | 6 | 7 | 0.42 0.16-0.22 0.06 0.59 0.00 |
| 37 | 1.327800 | 1.326699 | -0.08 | 1.00 | 3 | 6 | 0.26 0.34-0.18-0.01 0.53 0.05 |
| 38 | 0.000000 | 1.348207 | 0.00 | 0.00 | 2 | 5 | 0.35 0.07-0.06-0.03 0.56 0.11 |
| 39 | 1.347900 | 1.350157 | 0.17 | 1.00 | 8 | 5 | 0.35 0.07-0.06-0.03 0.55 0.11 |
| 40 | 0.000000 | 1.357941 | 0.00 | 0.00 | 5 | 6 | 0.47 0.48-0.21 0.02 0.09 0.16 |
| 41 | 1.376100 | 1.379103 | 0.22 | 1.00 | 8 | 6 | 0.31 0.08-0.08-0.01 0.61 0.09 |
| 42 | 1.379600 | 1.380238 | 0.05 | 1.00 | 2 | 6 | 0.31 0.08-0.08-0.01 0.61 0.09 |
| 43 | 1.381200 | 1.381144 | 0.00 | 1.00 | 5 | 7 | 0.47 0.52-0.25 0.01 0.04 0.22 |
| 44 | 1.399400 | 1.405947 | 0.47 | 1.00 | 2 | 7 | 0.37 0.05-0.09 0.02 0.45 0.21 |
| 45 | 1.400700 | 1.407057 | 0.45 | 1.00 | 8 | 7 | 0.36 0.05-0.09 0.02 0.46 0.20 |
| 46 | 1.406700 | 1.407796 | 0.08 | 1.00 | 7 | 7 | 0.31 0.11-0.09-0.01 0.04 0.63 |
| 47 | 1.408600 | 1.408933 | 0.02 | 1.00 | 1 | 7 | 0.31 0.12-0.09-0.01 0.04 0.63 |
| 48 | 1.452100 | 1.456082 | 0.27 | 1.00 | 4 | 6 | 0.30 0.03-0.01-0.03 0.68 0.03 |
| 49 | 1.470800 | 1.475846 | 0.34 | 1.00 | 1 | 8 | 0.37 0.40-0.23 0.01 0.32 0.13 |
| 50 | 1.471900 | 1.475939 | 0.27 | 1.00 | 7 | 8 | 0.35 0.39-0.22 0.01 0.34 0.14 |
| 51 | 1.478300 | 1.476313 | -0.13 | 1.00 | 4 | 7 | 0.24 0.09-0.10 0.03 0.67 0.07 |
| 52 | 1.485400 | 1.486815 | 0.10 | 1.00 | 3 | 7 | 0.50 0.69-0.50 0.07 0.15 0.09 |

Bulk Modulus= 2.280

| c11 | c22 | c33 | c23 | c13 | c12 | c44 | c55 | c66 |
|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| 4.2447 | 4.2447 | 4.8988 | 1.5448 | 1.5448 | 0.7277 | 1.1257 | 1.1257 | 0.4878 |

| d1 | d2 | d3 |
|---------|---------|---------|
| 0.46390 | 0.46300 | 0.31680 |

loop# 6 rms error= 0.3291 %, changed by -.0000009 %

length of gradient vector= 0.000000 blamb= 0.000600

| eigenvalues | eigenvectors |
|-------------|--------------------------------|
| 0.00153 | -0.36 0.43-0.62 0.53-0.12 0.05 |
| 0.02636 | -0.65-0.69 0.16 0.28-0.04 0.02 |
| 0.13898 | -0.56 0.15-0.25-0.76 0.10-0.05 |
| 0.50790 | -0.36 0.57 0.73 0.14 0.00 0.00 |
| 3.21485 | 0.01-0.01 0.05-0.17-0.97 0.15 |
| 14.46762 | 0.00 0.00 0.01-0.04 0.17 0.99 |

chisquare increased 2% by the following % changes in independent parameters

| | | | | | |
|-------|-------|-------|-------|-------|-------|
| -0.94 | -1.46 | -4.02 | -5.51 | 0.09 | 0.05 |
| 0.27 | -0.37 | 0.26 | 2.07 | -0.02 | -0.01 |
| -0.17 | 0.04 | -0.19 | 1.16 | 0.05 | 0.02 |

zircon 512 K cool
 free moduli are c11, c33, c23, c12, c44, c66
 using 12 order polynomials mass= 0.3167 gm rho= 4.646 gm/cc

| n | fex | fr | %err | wt | k | i | df/d(moduli) |
|----|----------|----------|-------|------|---|---|-------------------------------|
| 1 | 0.306630 | 0.304339 | -0.75 | 1.00 | 4 | 1 | 0.00 0.00 0.00 0.00 0.17 0.83 |
| 2 | 0.442080 | 0.442055 | -0.01 | 1.00 | 3 | 2 | 0.02 0.00-0.01 0.00 0.00 0.98 |
| 3 | 0.598040 | 0.600236 | 0.37 | 1.00 | 7 | 2 | 0.31 0.04-0.08 0.00 0.00 0.73 |
| 4 | 0.604320 | 0.601743 | -0.43 | 1.00 | 1 | 2 | 0.31 0.04-0.08 0.00 0.00 0.73 |
| 5 | 0.676480 | 0.677721 | 0.18 | 1.00 | 6 | 2 | 0.83 0.01-0.02-0.12 0.30 0.00 |
| 6 | 0.693300 | 0.691508 | -0.26 | 1.00 | 4 | 2 | 0.05 0.00 0.00-0.01 0.95 0.01 |
| 7 | 0.698890 | 0.699830 | 0.13 | 1.00 | 6 | 3 | 0.71 0.14-0.28 0.09 0.34 0.00 |
| 8 | 0.757190 | 0.760111 | 0.39 | 1.00 | 8 | 2 | 0.38 0.04-0.06-0.02 0.34 0.33 |
| 9 | 0.767390 | 0.761554 | -0.76 | 1.00 | 2 | 2 | 0.38 0.04-0.06-0.02 0.34 0.32 |
| 10 | 0.814520 | 0.816859 | 0.29 | 1.00 | 2 | 3 | 0.07 0.01-0.01 0.00 0.93 0.01 |
| 11 | 0.815910 | 0.817508 | 0.20 | 1.00 | 8 | 3 | 0.07 0.01-0.01 0.00 0.93 0.01 |
| 12 | 0.923920 | 0.926681 | 0.30 | 1.00 | 3 | 3 | 0.14 0.01-0.03 0.00 0.00 0.87 |
| 13 | 0.931740 | 0.932413 | 0.07 | 1.00 | 5 | 1 | 1.21 0.01-0.02-0.21 0.00 0.00 |
| 14 | 0.934570 | 0.935067 | 0.05 | 1.00 | 5 | 2 | 1.10 0.28-0.38 0.00 0.00 0.00 |
| 15 | 0.937890 | 0.937197 | -0.07 | 1.00 | 5 | 3 | 1.03 0.46-0.62 0.13 0.00 0.00 |
| 16 | 0.940240 | 0.942978 | 0.29 | 1.00 | 8 | 4 | 0.35 0.04-0.09 0.00 0.54 0.14 |
| 17 | 0.952640 | 0.943875 | -0.92 | 1.00 | 2 | 4 | 0.35 0.04-0.09 0.00 0.54 0.15 |
| 18 | 0.988130 | 0.989138 | 0.10 | 1.00 | 7 | 3 | 0.84 0.28-0.33 0.00 0.01 0.20 |
| 19 | 0.990410 | 0.990435 | 0.00 | 1.00 | 1 | 3 | 0.84 0.29-0.33 0.00 0.01 0.20 |
| 20 | 0.995870 | 0.996994 | 0.11 | 1.00 | 4 | 3 | 0.07 0.01-0.01 0.01 0.83 0.10 |
| 21 | 1.043100 | 1.046676 | 0.34 | 1.00 | 3 | 4 | 0.07 0.02-0.03 0.00 0.00 0.93 |
| 22 | 1.050600 | 1.049745 | -0.08 | 1.00 | 6 | 4 | 0.43 0.06-0.10 0.01 0.33 0.28 |
| 23 | 1.142500 | 1.142977 | 0.04 | 1.00 | 4 | 4 | 0.09 0.02-0.02-0.01 0.39 0.53 |
| 24 | 1.177000 | 1.170195 | -0.58 | 1.00 | 6 | 5 | 0.76 0.10-0.17-0.02 0.33 0.00 |
| 25 | 1.182100 | 1.182688 | 0.05 | 1.00 | 5 | 4 | 0.59 0.53-0.41 0.04 0.02 0.24 |
| 26 | 1.205600 | 1.205539 | -0.01 | 1.00 | 3 | 5 | 0.18 0.80-0.35 0.03 0.24 0.10 |
| 27 | 1.209500 | 1.209729 | 0.02 | 1.00 | 4 | 5 | 0.04 0.01-0.01 0.00 0.34 0.63 |
| 28 | 0.000000 | 1.213022 | 0.00 | 0.00 | 7 | 4 | 0.53 0.35-0.20-0.03 0.19 0.17 |
| 29 | 0.000000 | 1.213034 | 0.00 | 0.00 | 1 | 4 | 0.54 0.35-0.20-0.03 0.19 0.17 |
| 30 | 0.000000 | 1.268688 | 0.00 | 0.00 | 7 | 5 | 0.33 0.73-0.36 0.04 0.17 0.09 |
| 31 | 1.274100 | 1.269053 | -0.40 | 1.00 | 1 | 5 | 0.33 0.73-0.36 0.04 0.17 0.09 |
| 32 | 0.000000 | 1.284410 | 0.00 | 0.00 | 7 | 6 | 0.25 0.20-0.05-0.02 0.15 0.46 |
| 33 | 1.287300 | 1.285753 | -0.12 | 1.00 | 1 | 6 | 0.26 0.20-0.05-0.02 0.15 0.46 |
| 34 | 0.000000 | 1.287001 | 0.00 | 0.00 | 5 | 5 | 0.51 0.55-0.13-0.06 0.13 0.00 |
| 35 | 1.294100 | 1.287955 | -0.47 | 1.00 | 6 | 6 | 0.43 0.04-0.02-0.07 0.63 0.00 |
| 36 | 0.000000 | 1.303890 | 0.00 | 0.00 | 6 | 7 | 0.42 0.17-0.23 0.06 0.59 0.00 |
| 37 | 0.000000 | 1.321336 | 0.00 | 0.00 | 3 | 6 | 0.27 0.34-0.18-0.01 0.53 0.05 |
| 38 | 0.000000 | 1.343751 | 0.00 | 0.00 | 2 | 5 | 0.36 0.07-0.07-0.03 0.56 0.11 |
| 39 | 1.343000 | 1.345682 | 0.20 | 1.00 | 8 | 5 | 0.36 0.07-0.07-0.03 0.55 0.12 |
| 40 | 0.000000 | 1.353754 | 0.00 | 0.00 | 5 | 6 | 0.47 0.50-0.23 0.02 0.09 0.16 |
| 41 | 0.000000 | 1.374439 | 0.00 | 0.00 | 8 | 6 | 0.31 0.08-0.08-0.01 0.61 0.09 |
| 42 | 1.374300 | 1.375576 | 0.09 | 1.00 | 2 | 6 | 0.31 0.08-0.08-0.01 0.61 0.09 |
| 43 | 1.376200 | 1.376472 | 0.02 | 1.00 | 5 | 7 | 0.48 0.51-0.26 0.01 0.04 0.21 |
| 44 | 0.000000 | 1.402005 | 0.00 | 0.00 | 2 | 7 | 0.37 0.05-0.10 0.02 0.45 0.20 |
| 45 | 1.397000 | 1.403141 | 0.44 | 1.00 | 8 | 7 | 0.36 0.05-0.10 0.02 0.46 0.20 |
| 46 | 1.402100 | 1.404104 | 0.14 | 1.00 | 7 | 7 | 0.31 0.12-0.09-0.01 0.04 0.63 |
| 47 | 1.404800 | 1.405244 | 0.03 | 1.00 | 1 | 7 | 0.31 0.12-0.09-0.01 0.04 0.63 |
| 48 | 1.447000 | 1.451862 | 0.34 | 1.00 | 4 | 6 | 0.30 0.03-0.01-0.03 0.68 0.03 |
| 49 | 1.465000 | 1.470113 | 0.35 | 1.00 | 1 | 8 | 0.40 0.43-0.25 0.00 0.29 0.13 |
| 50 | 1.466200 | 1.470285 | 0.28 | 1.00 | 7 | 8 | 0.38 0.41-0.24 0.01 0.32 0.13 |
| 51 | 1.473100 | 1.472215 | -0.06 | 1.00 | 4 | 7 | 0.24 0.10-0.10 0.03 0.67 0.07 |
| 52 | 1.479300 | 1.479816 | 0.03 | 1.00 | 3 | 7 | 0.51 0.70-0.51 0.07 0.15 0.09 |

Bulk Modulus= 2.287

| c11 | c22 | c33 | c23 | c13 | c12 | c44 | c55 | c66 |
|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| 4.2193 | 4.2193 | 4.9066 | 1.5702 | 1.5702 | 0.7463 | 1.1189 | 1.1189 | 0.4856 |

| d1 | d2 | d3 |
|---------|---------|---------|
| 0.46400 | 0.46310 | 0.31720 |

loop# 5 rms error= 0.3336 %, changed by -.0000037 %

length of gradient vector= 0.000001 blamb= 0.000736

| eigenvalues | eigenvectors |
|-------------|--------------------------------|
| 0.00146 | -0.37-0.42-0.61-0.54-0.12 0.05 |
| 0.02383 | -0.64 0.69 0.16-0.28-0.03 0.02 |
| 0.14012 | -0.56-0.14-0.26 0.77 0.09-0.05 |
| 0.51964 | -0.37-0.57 0.72-0.13 0.01 0.00 |
| 2.79109 | 0.01 0.01 0.05 0.15-0.98 0.14 |
| 14.38882 | 0.00 0.00 0.01 0.05 0.15 0.99 |

chisquare increased 2% by the following % changes in independent parameters

| | | | | | |
|-------|-------|-------|-------|------|------|
| -0.95 | -1.43 | -3.90 | -5.42 | 0.09 | 0.05 |
| -0.27 | 0.38 | -0.24 | -2.04 | 0.02 | 0.01 |
| -0.16 | 0.04 | -0.19 | 1.08 | 0.05 | 0.02 |

zircon 607 K cool
 free moduli are c11, c33, c23, c12, c44, c66
 using 12 order polynomials mass= 0.3167 gm rho= 4.642 gm/cc

| n | fex | fr | %err | wt | k | i | df/d(moduli) |
|----|----------|----------|-------|------|---|---|-------------------------------|
| 1 | 0.306290 | 0.304261 | -0.66 | 1.00 | 4 | 1 | 0.00 0.00 0.00 0.00 0.17 0.82 |
| 2 | 0.441380 | 0.442357 | 0.22 | 1.00 | 3 | 2 | 0.02 0.00-0.01 0.00 0.00 0.98 |
| 3 | 0.596470 | 0.599447 | 0.50 | 1.00 | 7 | 2 | 0.31 0.04-0.08 0.00 0.00 0.72 |
| 4 | 0.602780 | 0.600955 | -0.30 | 1.00 | 1 | 2 | 0.31 0.04-0.08 0.00 0.00 0.72 |
| 5 | 0.673210 | 0.672281 | -0.14 | 1.00 | 6 | 2 | 0.84 0.01-0.02-0.13 0.30 0.00 |
| 6 | 0.690600 | 0.688709 | -0.27 | 1.00 | 4 | 2 | 0.05 0.00 0.00-0.01 0.95 0.01 |
| 7 | 0.695750 | 0.696207 | 0.07 | 1.00 | 6 | 3 | 0.71 0.14-0.27 0.09 0.34 0.00 |
| 8 | 0.754570 | 0.757127 | 0.34 | 1.00 | 8 | 2 | 0.38 0.04-0.06-0.02 0.34 0.32 |
| 9 | 0.764800 | 0.758551 | -0.82 | 1.00 | 2 | 2 | 0.39 0.04-0.06-0.02 0.34 0.32 |
| 10 | 0.811380 | 0.813407 | 0.25 | 1.00 | 2 | 3 | 0.07 0.01-0.01 0.00 0.93 0.01 |
| 11 | 0.812790 | 0.814050 | 0.16 | 1.00 | 8 | 3 | 0.07 0.01-0.01 0.00 0.93 0.01 |
| 12 | 0.921410 | 0.923269 | 0.20 | 1.00 | 5 | 1 | 1.22 0.00 0.00-0.22 0.00 0.00 |
| 13 | 0.926720 | 0.926482 | -0.03 | 1.00 | 3 | 3 | 0.15 0.01-0.03 0.00 0.00 0.87 |
| 14 | 0.929490 | 0.928766 | -0.08 | 1.00 | 5 | 2 | 1.10 0.27-0.36-0.01 0.00 0.00 |
| 15 | 0.933500 | 0.932948 | -0.06 | 1.00 | 5 | 3 | 1.02 0.47-0.63 0.14 0.00 0.00 |
| 16 | 0.936290 | 0.939041 | 0.29 | 1.00 | 8 | 4 | 0.35 0.04-0.08 0.00 0.54 0.15 |
| 17 | 0.948900 | 0.939942 | -0.94 | 1.00 | 2 | 4 | 0.35 0.04-0.08 0.00 0.54 0.15 |
| 18 | 0.983480 | 0.984157 | 0.07 | 1.00 | 7 | 3 | 0.83 0.27-0.32-0.01 0.01 0.20 |
| 19 | 0.985940 | 0.985442 | -0.05 | 1.00 | 1 | 3 | 0.83 0.28-0.32-0.01 0.01 0.20 |
| 20 | 0.992110 | 0.993259 | 0.12 | 1.00 | 4 | 3 | 0.07 0.01-0.01 0.01 0.83 0.10 |
| 21 | 1.041100 | 1.045545 | 0.43 | 1.00 | 6 | 4 | 0.43 0.05-0.10 0.00 0.33 0.28 |
| 22 | 1.046800 | 1.047003 | 0.02 | 1.00 | 3 | 4 | 0.08 0.02-0.03 0.00 0.00 0.92 |
| 23 | 1.139300 | 1.141022 | 0.15 | 1.00 | 4 | 4 | 0.09 0.02-0.02-0.01 0.39 0.53 |
| 24 | 1.171600 | 1.162955 | -0.74 | 1.00 | 6 | 5 | 0.75 0.10-0.17-0.02 0.34 0.00 |
| 25 | 1.176900 | 1.178086 | 0.10 | 1.00 | 5 | 4 | 0.59 0.52-0.41 0.04 0.02 0.24 |
| 26 | 1.200300 | 1.200380 | 0.01 | 1.00 | 3 | 5 | 0.18 0.80-0.34 0.03 0.24 0.10 |
| 27 | 1.206400 | 1.206712 | 0.03 | 1.00 | 1 | 4 | 0.53 0.36-0.20-0.03 0.19 0.16 |
| 28 | 0.000000 | 1.206718 | 0.00 | 0.00 | 7 | 4 | 0.53 0.35-0.20-0.03 0.19 0.16 |
| 29 | 1.208900 | 1.208361 | -0.04 | 1.00 | 4 | 5 | 0.04 0.01-0.01 0.00 0.34 0.63 |
| 30 | 0.000000 | 1.262798 | 0.00 | 0.00 | 7 | 5 | 0.32 0.73-0.35 0.03 0.18 0.09 |
| 31 | 1.268500 | 1.263154 | -0.42 | 1.00 | 1 | 5 | 0.32 0.73-0.35 0.03 0.18 0.08 |
| 32 | 1.274800 | 1.277718 | 0.23 | 1.00 | 5 | 5 | 0.51 0.56-0.13-0.06 0.13 0.00 |
| 33 | 1.281100 | 1.280162 | -0.07 | 1.00 | 6 | 6 | 0.42 0.04-0.02-0.07 0.63 0.00 |
| 34 | 0.000000 | 1.280284 | 0.00 | 0.00 | 7 | 6 | 0.27 0.20-0.05-0.02 0.14 0.46 |
| 35 | 1.289900 | 1.281563 | -0.65 | 1.00 | 1 | 6 | 0.28 0.21-0.05-0.02 0.14 0.45 |
| 36 | 0.000000 | 1.298217 | 0.00 | 0.00 | 6 | 7 | 0.41 0.16-0.23 0.06 0.59 0.00 |
| 37 | 1.317100 | 1.315186 | -0.15 | 1.00 | 3 | 6 | 0.27 0.34-0.18-0.01 0.53 0.05 |
| 38 | 1.336400 | 1.336982 | 0.04 | 1.00 | 2 | 5 | 0.36 0.07-0.06-0.04 0.56 0.11 |
| 39 | 1.337500 | 1.338939 | 0.11 | 1.00 | 8 | 5 | 0.36 0.07-0.06-0.04 0.55 0.11 |
| 40 | 0.000000 | 1.346974 | 0.00 | 0.00 | 5 | 6 | 0.47 0.48-0.22 0.02 0.09 0.16 |
| 41 | 0.000000 | 1.368065 | 0.00 | 0.00 | 8 | 6 | 0.31 0.08-0.08-0.01 0.61 0.09 |
| 42 | 1.368500 | 1.369204 | 0.05 | 1.00 | 2 | 6 | 0.31 0.08-0.08-0.01 0.61 0.09 |
| 43 | 1.370700 | 1.370014 | -0.05 | 1.00 | 5 | 7 | 0.47 0.52-0.26 0.01 0.04 0.22 |
| 44 | 1.389500 | 1.396461 | 0.50 | 1.00 | 2 | 7 | 0.37 0.05-0.09 0.02 0.45 0.21 |
| 45 | 1.392800 | 1.397596 | 0.34 | 1.00 | 8 | 7 | 0.36 0.05-0.09 0.02 0.45 0.21 |
| 46 | 1.397000 | 1.401394 | 0.31 | 1.00 | 7 | 7 | 0.30 0.12-0.09-0.01 0.03 0.64 |
| 47 | 1.400600 | 1.402578 | 0.14 | 1.00 | 1 | 7 | 0.30 0.12-0.09 0.00 0.03 0.64 |
| 48 | 1.441100 | 1.443928 | 0.20 | 1.00 | 4 | 6 | 0.31 0.03-0.01-0.03 0.68 0.03 |
| 49 | 1.458500 | 1.463087 | 0.31 | 1.00 | 1 | 8 | 0.44 0.48-0.27 0.00 0.24 0.11 |
| 50 | 1.460000 | 1.463439 | 0.24 | 1.00 | 7 | 8 | 0.42 0.45-0.26 0.00 0.26 0.12 |
| 51 | 1.467300 | 1.465892 | -0.10 | 1.00 | 4 | 7 | 0.24 0.09-0.10 0.03 0.67 0.07 |
| 52 | 1.472400 | 1.473817 | 0.10 | 1.00 | 3 | 7 | 0.51 0.69-0.51 0.07 0.15 0.09 |

Bulk Modulus= 2.251

| c11 | c22 | c33 | c23 | c13 | c12 | c44 | c55 | c66 |
|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| 4.1524 | 4.1524 | 4.8296 | 1.5350 | 1.5350 | 0.7477 | 1.1093 | 1.1093 | 0.4865 |

| d1 | d2 | d3 |
|---------|---------|---------|
| 0.46420 | 0.46330 | 0.31720 |

loop# 7 rms error= 0.3371 %, changed by -.0000001 %

length of gradient vector= 0.000000 blamb= 0.000633

| eigenvalues | eigenvectors |
|-------------|--------------------------------|
| 0.00221 | -0.38 0.45-0.58-0.54-0.13 0.06 |
| 0.03180 | -0.61-0.72 0.13-0.30-0.04 0.02 |
| 0.15872 | -0.57 0.11-0.28 0.76 0.10-0.05 |
| 0.55734 | -0.40 0.51 0.75-0.10 0.02 0.00 |
| 3.11511 | 0.01-0.01 0.06 0.17-0.97 0.16 |
| 14.57865 | 0.00 0.00 0.01 0.05 0.17 0.98 |

chisquare increased 2% by the following % changes in independent parameters

| | | | | | |
|-------|-------|-------|-------|-------|-------|
| -0.86 | -1.21 | -3.52 | -5.09 | 0.08 | 0.04 |
| 0.27 | -0.37 | 0.18 | 1.72 | -0.02 | -0.02 |
| -0.16 | 0.03 | -0.20 | 1.13 | 0.06 | 0.02 |

zircon 711 K cool
 free moduli are c11, c33, c23, c12, c44, c66
 using 12 order polynomials mass= 0.3167 gm rho= 4.638 gm/cc

| n | fex | fr | %err | wt | k | i | df/d(moduli) |
|----|----------|----------|-------|------|---|---|-------------------------------|
| 1 | 0.305450 | 0.303249 | -0.72 | 1.00 | 4 | 1 | 0.00 0.00 0.00 0.00 0.17 0.82 |
| 2 | 0.440590 | 0.440917 | 0.07 | 1.00 | 3 | 2 | 0.02 0.00-0.01 0.00 0.00 0.98 |
| 3 | 0.594690 | 0.597295 | 0.44 | 1.00 | 7 | 2 | 0.32 0.05-0.08 0.00 0.00 0.72 |
| 4 | 0.601130 | 0.598798 | -0.39 | 1.00 | 1 | 2 | 0.31 0.05-0.08 0.00 0.00 0.72 |
| 5 | 0.669650 | 0.669585 | -0.01 | 1.00 | 6 | 2 | 0.84 0.01-0.02-0.13 0.30 0.00 |
| 6 | 0.687750 | 0.685162 | -0.38 | 1.00 | 4 | 2 | 0.05 0.00 0.00-0.01 0.95 0.01 |
| 7 | 0.692410 | 0.693161 | 0.11 | 1.00 | 6 | 3 | 0.71 0.15-0.29 0.09 0.34 0.00 |
| 8 | 0.751670 | 0.754126 | 0.33 | 1.00 | 8 | 2 | 0.39 0.04-0.06-0.02 0.34 0.32 |
| 9 | 0.762080 | 0.755541 | -0.86 | 1.00 | 2 | 2 | 0.39 0.04-0.06-0.02 0.34 0.32 |
| 10 | 0.807930 | 0.809401 | 0.18 | 1.00 | 2 | 3 | 0.07 0.01-0.01 0.00 0.93 0.01 |
| 11 | 0.809370 | 0.810039 | 0.08 | 1.00 | 8 | 3 | 0.07 0.01-0.01 0.00 0.93 0.01 |
| 12 | 0.918270 | 0.919541 | 0.14 | 1.00 | 5 | 1 | 1.22 0.00-0.01-0.22 0.00 0.00 |
| 13 | 0.921260 | 0.923375 | 0.23 | 1.00 | 3 | 3 | 0.15 0.02-0.03 0.00 0.00 0.87 |
| 14 | 0.924080 | 0.923866 | -0.02 | 1.00 | 5 | 2 | 1.11 0.28-0.38-0.01 0.00 0.00 |
| 15 | 0.928890 | 0.927178 | -0.18 | 1.00 | 5 | 3 | 1.02 0.48-0.65 0.15 0.00 0.00 |
| 16 | 0.932060 | 0.934715 | 0.28 | 1.00 | 8 | 4 | 0.35 0.04-0.09 0.00 0.54 0.15 |
| 17 | 0.944870 | 0.935614 | -0.98 | 1.00 | 2 | 4 | 0.35 0.04-0.09 0.00 0.54 0.15 |
| 18 | 0.978430 | 0.979171 | 0.08 | 1.00 | 7 | 3 | 0.84 0.29-0.33 0.00 0.01 0.20 |
| 19 | 0.981040 | 0.980443 | -0.06 | 1.00 | 1 | 3 | 0.84 0.29-0.33 0.00 0.01 0.20 |
| 20 | 0.988030 | 0.988650 | 0.06 | 1.00 | 4 | 3 | 0.07 0.01-0.01 0.01 0.83 0.10 |
| 21 | 1.038900 | 1.041400 | 0.24 | 1.00 | 6 | 4 | 0.43 0.06-0.10 0.01 0.33 0.28 |
| 22 | 1.042600 | 1.043489 | 0.09 | 1.00 | 3 | 4 | 0.08 0.03-0.03 0.00 0.00 0.92 |
| 23 | 1.135700 | 1.136351 | 0.06 | 1.00 | 4 | 4 | 0.09 0.02-0.02-0.01 0.39 0.53 |
| 24 | 1.165700 | 1.157385 | -0.71 | 1.00 | 6 | 5 | 0.76 0.10-0.18-0.02 0.34 0.00 |
| 25 | 1.171200 | 1.172155 | 0.08 | 1.00 | 5 | 4 | 0.60 0.53-0.42 0.04 0.02 0.24 |
| 26 | 1.194500 | 1.195447 | 0.08 | 1.00 | 3 | 5 | 0.18 0.81-0.36 0.03 0.24 0.10 |
| 27 | 1.202600 | 1.201514 | -0.09 | 1.00 | 1 | 4 | 0.54 0.36-0.21-0.03 0.19 0.16 |
| 28 | 0.000000 | 1.201530 | 0.00 | 0.00 | 7 | 4 | 0.54 0.36-0.21-0.03 0.19 0.16 |
| 29 | 1.203500 | 1.203686 | 0.02 | 1.00 | 4 | 5 | 0.04 0.01-0.01 0.00 0.34 0.63 |
| 30 | 0.000000 | 1.257689 | 0.00 | 0.00 | 7 | 5 | 0.33 0.74-0.37 0.04 0.18 0.09 |
| 31 | 1.262500 | 1.258044 | -0.35 | 1.00 | 1 | 5 | 0.33 0.74-0.37 0.04 0.18 0.09 |
| 32 | 0.000000 | 1.274183 | 0.00 | 0.00 | 6 | 6 | 0.43 0.04-0.03-0.07 0.63 0.00 |
| 33 | 1.273200 | 1.274392 | 0.09 | 1.00 | 5 | 5 | 0.52 0.55-0.14-0.07 0.13 0.00 |
| 34 | 1.274500 | 1.276499 | 0.16 | 1.00 | 7 | 6 | 0.27 0.20-0.05-0.02 0.14 0.45 |
| 35 | 1.285100 | 1.277775 | -0.57 | 1.00 | 1 | 6 | 0.27 0.21-0.05-0.02 0.14 0.45 |
| 36 | 1.287900 | 1.291520 | 0.28 | 1.00 | 6 | 7 | 0.42 0.17-0.24 0.06 0.59 0.00 |
| 37 | 1.310800 | 1.308743 | -0.16 | 1.00 | 3 | 6 | 0.27 0.34-0.19-0.01 0.53 0.06 |
| 38 | 1.330500 | 1.330942 | 0.03 | 1.00 | 2 | 5 | 0.36 0.07-0.07-0.04 0.56 0.11 |
| 39 | 1.331600 | 1.332892 | 0.10 | 1.00 | 8 | 5 | 0.36 0.07-0.07-0.04 0.56 0.11 |
| 40 | 1.344000 | 1.342831 | -0.09 | 1.00 | 5 | 6 | 0.47 0.50-0.24 0.02 0.09 0.16 |
| 41 | 1.359400 | 1.361674 | 0.17 | 1.00 | 8 | 6 | 0.31 0.08-0.08-0.01 0.61 0.09 |
| 42 | 1.362100 | 1.362812 | 0.05 | 1.00 | 2 | 6 | 0.31 0.08-0.08-0.01 0.61 0.09 |
| 43 | 1.364600 | 1.365342 | 0.05 | 1.00 | 5 | 7 | 0.49 0.50-0.26 0.01 0.04 0.22 |
| 44 | 1.383800 | 1.390744 | 0.50 | 1.00 | 2 | 7 | 0.37 0.05-0.10 0.02 0.45 0.21 |
| 45 | 1.388300 | 1.391880 | 0.26 | 1.00 | 8 | 7 | 0.36 0.05-0.10 0.02 0.45 0.21 |
| 46 | 1.391400 | 1.396392 | 0.36 | 1.00 | 7 | 7 | 0.31 0.13-0.10 0.00 0.04 0.64 |
| 47 | 1.396100 | 1.397560 | 0.10 | 1.00 | 1 | 7 | 0.30 0.13-0.10 0.00 0.04 0.64 |
| 48 | 1.434700 | 1.437862 | 0.22 | 1.00 | 4 | 6 | 0.31 0.03-0.01-0.04 0.68 0.03 |
| 49 | 1.451300 | 1.456551 | 0.36 | 1.00 | 1 | 8 | 0.45 0.47-0.28 0.00 0.24 0.12 |
| 50 | 1.452900 | 1.456884 | 0.27 | 1.00 | 7 | 8 | 0.43 0.45-0.27 0.00 0.26 0.12 |
| 51 | 1.460800 | 1.459334 | -0.10 | 1.00 | 4 | 7 | 0.25 0.10-0.11 0.03 0.67 0.07 |
| 52 | 1.464900 | 1.465697 | 0.05 | 1.00 | 3 | 7 | 0.51 0.70-0.53 0.07 0.15 0.09 |

Bulk Modulus= 2.266

| c11 | c22 | c33 | c23 | c13 | c12 | c44 | c55 | c66 |
|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| 4.1399 | 4.1399 | 4.8497 | 1.5715 | 1.5715 | 0.7646 | 1.0979 | 1.0979 | 0.4830 |

| d1 | d2 | d3 |
|---------|---------|---------|
| 0.46430 | 0.46340 | 0.31740 |

loop#20 rms error= 0.3270 %, changed by 0.0000417 %

length of gradient vector= 0.000138 blamb= 0.011764

| eigenvalues | eigenvectors |
|-------------|--------------------------------|
| 0.00541 | -0.37 0.46-0.59 0.54-0.13 0.06 |
| 0.03401 | -0.62-0.71 0.12 0.30-0.04 0.02 |
| 0.16172 | -0.56 0.12-0.27-0.76 0.11-0.05 |
| 0.60137 | -0.40 0.52 0.75 0.11 0.00 0.00 |
| 3.34776 | 0.01-0.01 0.04-0.18-0.97 0.16 |
| 15.47702 | 0.00 0.00 0.01-0.05 0.17 0.98 |

chisquare increased 2% by the following % changes in independent parameters

| | | | | | |
|-------|-------|-------|-------|-------|-------|
| -0.54 | -0.78 | -2.19 | -3.21 | 0.05 | 0.03 |
| 0.27 | -0.36 | 0.19 | 1.64 | -0.03 | -0.01 |
| -0.16 | 0.03 | -0.19 | 1.09 | 0.04 | 0.03 |

zircon 823 K cool
 free moduli are c11, c33, c23, c12, c44, c66
 using 12 order polynomials mass= 0.3167 gm rho= 4.631 gm/cc

| n | fex | fr | %err | wt | k | i | df/d(moduli) |
|----|----------|----------|-------|------|---|---|-------------------------------|
| 1 | 0.305010 | 0.302437 | -0.84 | 1.00 | 4 | 1 | 0.00 0.00 0.00 0.00 0.17 0.82 |
| 2 | 0.439680 | 0.439771 | 0.02 | 1.00 | 3 | 2 | 0.02 0.00-0.01 0.00 0.00 0.98 |
| 3 | 0.592760 | 0.595255 | 0.42 | 1.00 | 7 | 2 | 0.32 0.05-0.08 0.00 0.00 0.72 |
| 4 | 0.599240 | 0.596753 | -0.41 | 1.00 | 1 | 2 | 0.32 0.05-0.08 0.00 0.00 0.72 |
| 5 | 0.665810 | 0.666031 | 0.03 | 1.00 | 6 | 2 | 0.84 0.01-0.02-0.13 0.30 0.00 |
| 6 | 0.684530 | 0.682380 | -0.31 | 1.00 | 4 | 2 | 0.05 0.00 0.00-0.01 0.95 0.01 |
| 7 | 0.688670 | 0.689822 | 0.17 | 1.00 | 6 | 3 | 0.72 0.15-0.29 0.09 0.34 0.00 |
| 8 | 0.000000 | 0.751085 | 0.00 | 0.00 | 8 | 2 | 0.39 0.04-0.06-0.02 0.34 0.32 |
| 9 | 0.758920 | 0.752490 | -0.85 | 1.00 | 2 | 2 | 0.39 0.04-0.06-0.02 0.34 0.32 |
| 10 | 0.804140 | 0.806138 | 0.25 | 1.00 | 2 | 3 | 0.07 0.01-0.01 0.00 0.93 0.01 |
| 11 | 0.805600 | 0.806774 | 0.15 | 1.00 | 8 | 3 | 0.07 0.01-0.01 0.00 0.93 0.01 |
| 12 | 0.914120 | 0.913916 | -0.02 | 1.00 | 5 | 1 | 1.23 0.00-0.01-0.22 0.00 0.00 |
| 13 | 0.915660 | 0.918570 | 0.32 | 1.00 | 5 | 2 | 1.11 0.28-0.38-0.01 0.00 0.00 |
| 14 | 0.918330 | 0.920650 | 0.25 | 1.00 | 3 | 3 | 0.15 0.02-0.03 0.00 0.00 0.87 |
| 15 | 0.924450 | 0.922120 | -0.25 | 1.00 | 5 | 3 | 1.02 0.48-0.65 0.15 0.00 0.00 |
| 16 | 0.927510 | 0.930708 | 0.34 | 1.00 | 8 | 4 | 0.35 0.04-0.09 0.00 0.54 0.15 |
| 17 | 0.940430 | 0.931605 | -0.94 | 1.00 | 2 | 4 | 0.35 0.04-0.09 0.00 0.54 0.15 |
| 18 | 0.972990 | 0.974200 | 0.12 | 1.00 | 7 | 3 | 0.84 0.28-0.33 0.00 0.01 0.20 |
| 19 | 0.975710 | 0.975461 | -0.03 | 1.00 | 1 | 3 | 0.84 0.29-0.33 0.00 0.01 0.20 |
| 20 | 0.983610 | 0.984818 | 0.12 | 1.00 | 4 | 3 | 0.07 0.01-0.02 0.01 0.83 0.10 |
| 21 | 1.036400 | 1.037104 | 0.07 | 1.00 | 6 | 4 | 0.43 0.06-0.10 0.00 0.33 0.28 |
| 22 | 1.038200 | 1.040596 | 0.23 | 1.00 | 3 | 4 | 0.08 0.03-0.03 0.00 0.00 0.92 |
| 23 | 1.131700 | 1.132541 | 0.07 | 1.00 | 4 | 4 | 0.09 0.02-0.02-0.01 0.39 0.53 |
| 24 | 1.159300 | 1.151416 | -0.68 | 1.00 | 6 | 5 | 0.76 0.10-0.18-0.02 0.34 0.00 |
| 25 | 1.165100 | 1.166354 | 0.11 | 1.00 | 5 | 4 | 0.59 0.53-0.42 0.04 0.02 0.24 |
| 26 | 1.188300 | 1.189269 | 0.08 | 1.00 | 3 | 5 | 0.18 0.81-0.36 0.03 0.24 0.10 |
| 27 | 1.196500 | 1.195467 | -0.09 | 1.00 | 1 | 4 | 0.54 0.36-0.21-0.03 0.19 0.16 |
| 28 | 0.000000 | 1.195491 | 0.00 | 0.00 | 7 | 4 | 0.54 0.36-0.21-0.03 0.19 0.16 |
| 29 | 1.199500 | 1.199927 | 0.04 | 1.00 | 4 | 5 | 0.04 0.01-0.01 0.00 0.34 0.63 |
| 30 | 0.000000 | 1.251071 | 0.00 | 0.00 | 7 | 5 | 0.33 0.74-0.37 0.04 0.18 0.09 |
| 31 | 1.255800 | 1.251422 | -0.35 | 1.00 | 1 | 5 | 0.33 0.74-0.37 0.04 0.18 0.09 |
| 32 | 0.000000 | 1.267007 | 0.00 | 0.00 | 5 | 5 | 0.52 0.55-0.14-0.07 0.13 0.00 |
| 33 | 0.000000 | 1.268189 | 0.00 | 0.00 | 6 | 6 | 0.42 0.04-0.03-0.07 0.63 0.00 |
| 34 | 1.267500 | 1.271219 | 0.29 | 1.00 | 7 | 6 | 0.27 0.20-0.05-0.02 0.14 0.45 |
| 35 | 1.279600 | 1.272467 | -0.56 | 1.00 | 1 | 6 | 0.28 0.21-0.05-0.02 0.14 0.45 |
| 36 | 1.288180 | 1.285670 | -0.19 | 1.00 | 6 | 7 | 0.42 0.17-0.24 0.06 0.59 0.00 |
| 37 | 1.304100 | 1.302544 | -0.12 | 1.00 | 3 | 6 | 0.27 0.34-0.19-0.01 0.53 0.06 |
| 38 | 1.324000 | 1.325107 | 0.08 | 1.00 | 2 | 5 | 0.36 0.07-0.06-0.04 0.56 0.11 |
| 39 | 1.325100 | 1.327052 | 0.15 | 1.00 | 8 | 5 | 0.36 0.07-0.07-0.04 0.56 0.11 |
| 40 | 0.000000 | 1.335944 | 0.00 | 0.00 | 5 | 6 | 0.46 0.50-0.24 0.02 0.09 0.17 |
| 41 | 1.352700 | 1.355772 | 0.23 | 1.00 | 8 | 6 | 0.31 0.08-0.08-0.01 0.62 0.09 |
| 42 | 1.355200 | 1.356906 | 0.13 | 1.00 | 2 | 6 | 0.31 0.08-0.08-0.01 0.61 0.09 |
| 43 | 1.358000 | 1.358441 | 0.03 | 1.00 | 5 | 7 | 0.48 0.50-0.26 0.01 0.04 0.22 |
| 44 | 1.377600 | 1.384961 | 0.53 | 1.00 | 2 | 7 | 0.37 0.05-0.10 0.02 0.45 0.21 |
| 45 | 1.383200 | 1.386101 | 0.21 | 1.00 | 8 | 7 | 0.36 0.05-0.10 0.02 0.45 0.21 |
| 46 | 1.385400 | 1.391288 | 0.42 | 1.00 | 7 | 7 | 0.30 0.13-0.10 0.00 0.04 0.64 |
| 47 | 1.391000 | 1.392462 | 0.11 | 1.00 | 1 | 7 | 0.30 0.14-0.11 0.00 0.04 0.64 |
| 48 | 1.427700 | 1.431529 | 0.27 | 1.00 | 4 | 6 | 0.31 0.03-0.01-0.04 0.67 0.03 |
| 49 | 0.000000 | 1.449173 | 0.00 | 0.00 | 1 | 8 | 0.48 0.49-0.29-0.01 0.21 0.11 |
| 50 | 1.445300 | 1.449599 | 0.30 | 1.00 | 7 | 8 | 0.45 0.48-0.28 0.00 0.23 0.12 |
| 51 | 1.453800 | 1.453222 | -0.04 | 1.00 | 4 | 7 | 0.25 0.10-0.11 0.03 0.66 0.07 |
| 52 | 1.456900 | 1.458167 | 0.09 | 1.00 | 3 | 7 | 0.51 0.70-0.53 0.07 0.15 0.09 |

Bulk Modulus= 2.239

| c11 | c22 | c33 | c23 | c13 | c12 | c44 | c55 | c66 |
|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| 4.0902 | 4.0902 | 4.7900 | 1.5523 | 1.5523 | 0.7583 | 1.0889 | 1.0889 | 0.4803 |

| d1 | d2 | d3 |
|---------|---------|---------|
| 0.46450 | 0.46360 | 0.31760 |

loop# 6 rms error= 0.3464 %, changed by 0.000003 %

length of gradient vector= 0.000001 blamb= 0.000793

| eigenvalues | eigenvectors |
|-------------|--------------------------------|
| 0.00181 | -0.36 0.45-0.60 0.54-0.12 0.06 |
| 0.02817 | -0.65-0.69 0.14 0.28-0.04 0.02 |
| 0.15804 | -0.56 0.15-0.26-0.76 0.11-0.05 |
| 0.57154 | -0.37 0.54 0.74 0.13 0.00 0.00 |
| 3.29729 | 0.01-0.01 0.04-0.17-0.97 0.15 |
| 15.09851 | 0.00 0.00 0.01-0.05 0.17 0.98 |

chisquare increased 2% by the following % changes in independent parameters

| | | | | | |
|-------|-------|-------|-------|-------|------|
| -0.95 | -1.44 | -3.85 | -5.23 | 0.09 | 0.06 |
| 0.30 | -0.39 | 0.26 | 1.94 | -0.03 | 0.00 |
| -0.17 | 0.03 | -0.19 | 1.12 | 0.04 | 0.03 |

zircon 939 K cool
 free moduli are c11, c33, c23, c12, c44, c66
 using 12 order polynomials mass= 0.3167 gm rho= 4.622 gm/cc

| n | fex | fr | %err | wt | k | i | df/d(moduli) |
|----|----------|----------|-------|------|---|---|-------------------------------|
| 1 | 0.304280 | 0.301877 | -0.79 | 1.00 | 4 | 1 | 0.00 0.00 0.00 0.00 0.17 0.82 |
| 2 | 0.438660 | 0.439070 | 0.09 | 1.00 | 3 | 2 | 0.02 0.00-0.01 0.00 0.00 0.98 |
| 3 | 0.590670 | 0.593376 | 0.46 | 1.00 | 7 | 2 | 0.32 0.05-0.09 0.00 0.00 0.71 |
| 4 | 0.597180 | 0.594871 | -0.39 | 1.00 | 1 | 2 | 0.32 0.05-0.09 0.00 0.00 0.72 |
| 5 | 0.661750 | 0.662504 | 0.11 | 1.00 | 6 | 2 | 0.85 0.01-0.02-0.13 0.30 0.00 |
| 6 | 0.681030 | 0.678717 | -0.34 | 1.00 | 4 | 2 | 0.05 0.00 0.00-0.01 0.95 0.01 |
| 7 | 0.684720 | 0.685012 | 0.04 | 1.00 | 6 | 3 | 0.72 0.15-0.30 0.09 0.33 0.00 |
| 8 | 0.000000 | 0.747860 | 0.00 | 0.00 | 8 | 2 | 0.39 0.04-0.07-0.02 0.34 0.32 |
| 9 | 0.755540 | 0.749252 | -0.83 | 1.00 | 2 | 2 | 0.39 0.04-0.07-0.02 0.34 0.32 |
| 10 | 0.800080 | 0.801898 | 0.23 | 1.00 | 2 | 3 | 0.07 0.01-0.01 0.00 0.93 0.01 |
| 11 | 0.801550 | 0.802530 | 0.12 | 1.00 | 8 | 3 | 0.07 0.01-0.01 0.00 0.93 0.01 |
| 12 | 0.908520 | 0.908791 | 0.03 | 1.00 | 5 | 1 | 1.22 0.01-0.02-0.22 0.00 0.00 |
| 13 | 0.910140 | 0.911311 | 0.13 | 1.00 | 5 | 2 | 1.11 0.29-0.40 0.00 0.00 0.00 |
| 14 | 0.912470 | 0.913340 | 0.10 | 1.00 | 5 | 3 | 1.03 0.48-0.66 0.14 0.00 0.00 |
| 15 | 0.919900 | 0.918608 | -0.14 | 1.00 | 3 | 3 | 0.15 0.02-0.03 0.00 0.00 0.86 |
| 16 | 0.922750 | 0.925694 | 0.32 | 1.00 | 8 | 4 | 0.35 0.05-0.09 0.00 0.54 0.15 |
| 17 | 0.935930 | 0.926592 | -1.00 | 1.00 | 2 | 4 | 0.35 0.05-0.09 0.00 0.54 0.15 |
| 18 | 0.967230 | 0.967712 | 0.05 | 1.00 | 7 | 3 | 0.83 0.29-0.34 0.00 0.01 0.21 |
| 19 | 0.970110 | 0.968954 | -0.12 | 1.00 | 1 | 3 | 0.83 0.30-0.35 0.00 0.01 0.21 |
| 20 | 0.978930 | 0.980039 | 0.11 | 1.00 | 4 | 3 | 0.07 0.01-0.02 0.01 0.82 0.10 |
| 21 | 1.033320 | 1.032241 | -0.10 | 1.00 | 6 | 4 | 0.43 0.06-0.11 0.01 0.33 0.28 |
| 22 | 1.033800 | 1.038548 | 0.46 | 1.00 | 3 | 4 | 0.08 0.03-0.03 0.00 0.00 0.92 |
| 23 | 1.127300 | 1.128687 | 0.12 | 1.00 | 4 | 4 | 0.09 0.02-0.02-0.01 0.38 0.53 |
| 24 | 1.152500 | 1.143816 | -0.75 | 1.00 | 6 | 5 | 0.76 0.11-0.18-0.02 0.34 0.00 |
| 25 | 1.158600 | 1.158782 | 0.02 | 1.00 | 5 | 4 | 0.60 0.55-0.44 0.04 0.02 0.24 |
| 26 | 1.181800 | 1.182664 | 0.07 | 1.00 | 3 | 5 | 0.19 0.82-0.38 0.03 0.23 0.10 |
| 27 | 0.000000 | 1.188878 | 0.00 | 0.00 | 1 | 4 | 0.55 0.37-0.22-0.03 0.18 0.16 |
| 28 | 0.000000 | 1.188920 | 0.00 | 0.00 | 7 | 4 | 0.55 0.37-0.22-0.03 0.19 0.16 |
| 29 | 1.195500 | 1.196443 | 0.08 | 1.00 | 4 | 5 | 0.04 0.01-0.01 0.00 0.34 0.63 |
| 30 | 0.000000 | 1.243778 | 0.00 | 0.00 | 7 | 5 | 0.34 0.74-0.38 0.04 0.18 0.09 |
| 31 | 1.249400 | 1.244121 | -0.42 | 1.00 | 1 | 5 | 0.34 0.74-0.38 0.04 0.18 0.09 |
| 32 | 0.000000 | 1.261113 | 0.00 | 0.00 | 5 | 5 | 0.52 0.55-0.14-0.07 0.13 0.00 |
| 33 | 1.258700 | 1.261391 | 0.21 | 1.00 | 6 | 6 | 0.42 0.04-0.03-0.07 0.63 0.00 |
| 34 | 0.000000 | 1.266987 | 0.00 | 0.00 | 7 | 6 | 0.28 0.21-0.06-0.02 0.14 0.44 |
| 35 | 1.273100 | 1.268200 | -0.38 | 1.00 | 1 | 6 | 0.29 0.21-0.06-0.02 0.14 0.44 |
| 36 | 1.275800 | 1.277012 | 0.09 | 1.00 | 6 | 7 | 0.42 0.17-0.25 0.06 0.59 0.00 |
| 37 | 1.296900 | 1.295056 | -0.14 | 1.00 | 3 | 6 | 0.28 0.35-0.20-0.01 0.53 0.06 |
| 38 | 1.317100 | 1.318399 | 0.10 | 1.00 | 2 | 5 | 0.36 0.08-0.07-0.04 0.56 0.10 |
| 39 | 1.318200 | 1.320348 | 0.16 | 1.00 | 8 | 5 | 0.36 0.08-0.07-0.04 0.56 0.11 |
| 40 | 0.000000 | 1.329152 | 0.00 | 0.00 | 5 | 6 | 0.46 0.52-0.26 0.02 0.09 0.17 |
| 41 | 1.345000 | 1.348522 | 0.26 | 1.00 | 8 | 6 | 0.31 0.08-0.09-0.01 0.62 0.09 |
| 42 | 1.347000 | 1.349654 | 0.20 | 1.00 | 2 | 6 | 0.31 0.08-0.09-0.01 0.62 0.09 |
| 43 | 1.350900 | 1.351574 | 0.05 | 1.00 | 5 | 7 | 0.49 0.49-0.26 0.01 0.05 0.22 |
| 44 | 1.371000 | 1.378024 | 0.51 | 1.00 | 2 | 7 | 0.37 0.05-0.11 0.02 0.44 0.21 |
| 45 | 1.377600 | 1.379170 | 0.11 | 1.00 | 8 | 7 | 0.37 0.05-0.10 0.02 0.45 0.21 |
| 46 | 1.379200 | 1.386585 | 0.54 | 1.00 | 7 | 7 | 0.30 0.15-0.12 0.00 0.04 0.63 |
| 47 | 1.385600 | 1.387752 | 0.16 | 1.00 | 1 | 7 | 0.30 0.15-0.12 0.00 0.04 0.63 |
| 48 | 1.420300 | 1.424488 | 0.29 | 1.00 | 4 | 6 | 0.31 0.03-0.01-0.04 0.67 0.03 |
| 49 | 1.435200 | 1.440788 | 0.39 | 0.00 | 1 | 8 | 0.50 0.50-0.29-0.01 0.19 0.12 |
| 50 | 1.437200 | 1.441252 | 0.28 | 1.00 | 7 | 8 | 0.48 0.48-0.29-0.01 0.21 0.12 |
| 51 | 1.446200 | 1.445401 | -0.06 | 1.00 | 4 | 7 | 0.25 0.10-0.11 0.03 0.66 0.07 |
| 52 | 1.448500 | 1.447450 | -0.07 | 1.00 | 3 | 7 | 0.52 0.70-0.54 0.08 0.15 0.09 |

Bulk Modulus= 2.229

| c11 | c22 | c33 | c23 | c13 | c12 | c44 | c55 | c66 |
|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| 4.0464 | 4.0464 | 4.7784 | 1.5687 | 1.5687 | 0.7544 | 1.0772 | 1.0772 | 0.4784 |

| d1 | d2 | d3 |
|---------|---------|---------|
| 0.46470 | 0.46380 | 0.31790 |

loop#20 rms error= 0.3512 %, changed by 0.0002102 %

length of gradient vector= 0.000428 blamb= 0.020683

| eigenvalues | eigenvectors |
|-------------|--------------------------------|
| 0.00587 | 0.32 0.46-0.62-0.53-0.12 0.05 |
| 0.03018 | 0.70-0.64 0.14-0.28-0.03 0.02 |
| 0.16331 | 0.54 0.20-0.26 0.77 0.10-0.05 |
| 0.59559 | 0.33 0.59 0.73-0.14 0.01 0.00 |
| 3.59708 | -0.01-0.01 0.05 0.16-0.97 0.16 |
| 14.90799 | 0.00 0.00 0.01 0.05 0.17 0.98 |

chisquare increased 2% by the following % changes in independent parameters

| | | | | | |
|-------|-------|-------|------|-------|-------|
| 0.48 | 0.87 | 2.04 | 2.62 | -0.04 | -0.03 |
| 0.30 | -0.35 | 0.33 | 2.03 | -0.02 | -0.01 |
| -0.17 | 0.03 | -0.19 | 1.09 | 0.05 | 0.02 |

zircon 1056 K cool
 free moduli are c11, c33, c23, c12, c44, c66
 using 12 order polynomials mass= 0.3167 gm rho= 4.616 gm/cc

| n | fex | fr | %err | wt | k | i | df/d(moduli) |
|----|----------|----------|-------|------|---|---|-------------------------------|
| 1 | 0.303810 | 0.300953 | -0.94 | 1.00 | 4 | 1 | 0.00 0.00 0.00 0.00 0.17 0.82 |
| 2 | 0.437530 | 0.437695 | 0.04 | 1.00 | 3 | 2 | 0.02 0.00-0.01 0.00 0.00 0.98 |
| 3 | 0.588470 | 0.591094 | 0.45 | 1.00 | 7 | 2 | 0.33 0.05-0.09 0.00 0.00 0.71 |
| 4 | 0.595090 | 0.592254 | -0.48 | 1.00 | 1 | 2 | 0.33 0.05-0.09 0.00 0.00 0.71 |
| 5 | 0.657520 | 0.658166 | 0.10 | 1.00 | 6 | 2 | 0.85 0.01-0.02-0.13 0.30 0.00 |
| 6 | 0.677420 | 0.674871 | -0.38 | 1.00 | 4 | 2 | 0.05 0.00 0.00-0.01 0.95 0.01 |
| 7 | 0.680740 | 0.681098 | 0.05 | 1.00 | 6 | 3 | 0.72 0.15-0.30 0.09 0.33 0.00 |
| 8 | 0.741520 | 0.744331 | 0.38 | 1.00 | 8 | 2 | 0.40 0.04-0.07-0.02 0.34 0.32 |
| 9 | 0.752060 | 0.745403 | -0.89 | 1.00 | 2 | 2 | 0.40 0.04-0.07-0.02 0.34 0.32 |
| 10 | 0.795870 | 0.797580 | 0.21 | 1.00 | 2 | 3 | 0.07 0.01-0.01 0.00 0.93 0.01 |
| 11 | 0.797340 | 0.798068 | 0.09 | 1.00 | 8 | 3 | 0.07 0.01-0.01 0.00 0.93 0.01 |
| 12 | 0.902190 | 0.901879 | -0.03 | 1.00 | 5 | 1 | 1.23 0.00-0.01-0.23 0.00 0.00 |
| 13 | 0.000000 | 0.905382 | 0.00 | 0.00 | 5 | 2 | 1.11 0.29-0.39-0.01 0.00 0.00 |
| 14 | 0.906890 | 0.908047 | 0.13 | 1.00 | 5 | 3 | 1.03 0.49-0.67 0.15 0.00 0.00 |
| 15 | 0.915890 | 0.915322 | -0.06 | 1.00 | 3 | 3 | 0.15 0.02-0.03 0.00 0.00 0.86 |
| 16 | 0.917800 | 0.920628 | 0.31 | 1.00 | 8 | 4 | 0.35 0.05-0.09 0.00 0.54 0.15 |
| 17 | 0.931190 | 0.921326 | -1.06 | 1.00 | 2 | 4 | 0.35 0.05-0.09 0.00 0.54 0.15 |
| 18 | 0.961350 | 0.962319 | 0.10 | 1.00 | 7 | 3 | 0.83 0.29-0.34 0.00 0.01 0.21 |
| 19 | 0.964310 | 0.963278 | -0.11 | 1.00 | 1 | 3 | 0.83 0.29-0.34 0.00 0.01 0.21 |
| 20 | 0.973960 | 0.974948 | 0.10 | 1.00 | 4 | 3 | 0.07 0.01-0.02 0.01 0.82 0.11 |
| 21 | 1.028300 | 1.027071 | -0.12 | 1.00 | 6 | 4 | 0.43 0.06-0.11 0.01 0.33 0.28 |
| 22 | 1.030800 | 1.035085 | 0.42 | 1.00 | 3 | 4 | 0.08 0.03-0.03 0.00 0.00 0.92 |
| 23 | 1.122700 | 1.123838 | 0.10 | 1.00 | 4 | 4 | 0.09 0.02-0.02-0.01 0.38 0.53 |
| 24 | 1.144300 | 1.136448 | -0.69 | 1.00 | 6 | 5 | 0.76 0.11-0.18-0.02 0.34 0.00 |
| 25 | 1.151900 | 1.152476 | 0.05 | 1.00 | 5 | 4 | 0.59 0.54-0.43 0.04 0.02 0.24 |
| 26 | 1.175100 | 1.175353 | 0.02 | 1.00 | 3 | 5 | 0.19 0.81-0.37 0.03 0.23 0.10 |
| 27 | 0.000000 | 1.181594 | 0.00 | 0.00 | 1 | 4 | 0.54 0.37-0.22-0.03 0.19 0.15 |
| 28 | 0.000000 | 1.181628 | 0.00 | 0.00 | 7 | 4 | 0.54 0.37-0.22-0.03 0.19 0.16 |
| 29 | 1.191200 | 1.191687 | 0.04 | 1.00 | 4 | 5 | 0.04 0.01-0.01 0.00 0.34 0.63 |
| 30 | 0.000000 | 1.236014 | 0.00 | 0.00 | 7 | 5 | 0.33 0.74-0.37 0.04 0.18 0.09 |
| 31 | 1.241300 | 1.236278 | -0.40 | 1.00 | 1 | 5 | 0.33 0.74-0.37 0.04 0.18 0.09 |
| 32 | 0.000000 | 1.251570 | 0.00 | 0.00 | 5 | 5 | 0.52 0.55-0.14-0.07 0.13 0.00 |
| 33 | 1.251100 | 1.253729 | 0.21 | 1.00 | 6 | 6 | 0.42 0.04-0.03-0.07 0.63 0.00 |
| 34 | 1.254700 | 1.260234 | 0.44 | 1.00 | 7 | 6 | 0.29 0.21-0.06-0.02 0.14 0.44 |
| 35 | 1.265900 | 1.261148 | -0.38 | 1.00 | 1 | 6 | 0.30 0.21-0.06-0.02 0.14 0.44 |
| 36 | 1.270000 | 1.269897 | -0.01 | 1.00 | 6 | 7 | 0.41 0.17-0.24 0.06 0.59 0.00 |
| 37 | 0.000000 | 1.287359 | 0.00 | 0.00 | 3 | 6 | 0.28 0.35-0.19-0.01 0.53 0.06 |
| 38 | 1.310000 | 1.311392 | 0.11 | 1.00 | 2 | 5 | 0.36 0.07-0.07-0.04 0.56 0.10 |
| 39 | 1.311100 | 1.312906 | 0.14 | 1.00 | 8 | 5 | 0.36 0.07-0.07-0.04 0.56 0.11 |
| 40 | 0.000000 | 1.320681 | 0.00 | 0.00 | 5 | 6 | 0.47 0.50-0.25 0.02 0.09 0.17 |
| 41 | 1.338200 | 1.341197 | 0.22 | 1.00 | 8 | 6 | 0.31 0.08-0.09-0.01 0.62 0.09 |
| 42 | 1.340500 | 1.342074 | 0.12 | 1.00 | 2 | 6 | 0.31 0.08-0.09-0.01 0.62 0.09 |
| 43 | 1.343500 | 1.343234 | -0.02 | 1.00 | 5 | 7 | 0.49 0.50-0.26 0.01 0.04 0.22 |
| 44 | 1.364100 | 1.370902 | 0.50 | 1.00 | 2 | 7 | 0.37 0.05-0.10 0.02 0.44 0.21 |
| 45 | 1.371300 | 1.371791 | 0.04 | 1.00 | 8 | 7 | 0.37 0.05-0.10 0.02 0.44 0.21 |
| 46 | 1.373100 | 1.380635 | 0.55 | 1.00 | 7 | 7 | 0.30 0.15-0.12 0.00 0.04 0.63 |
| 47 | 1.379900 | 1.381550 | 0.12 | 1.00 | 1 | 7 | 0.30 0.15-0.12 0.00 0.04 0.64 |
| 48 | 1.412500 | 1.416360 | 0.27 | 1.00 | 4 | 6 | 0.32 0.03-0.01-0.04 0.67 0.03 |
| 49 | 0.000000 | 1.432064 | 0.00 | 0.00 | 1 | 8 | 0.51 0.51-0.29-0.01 0.17 0.12 |
| 50 | 1.428700 | 1.432466 | 0.26 | 1.00 | 7 | 8 | 0.50 0.50-0.29-0.01 0.18 0.12 |
| 51 | 1.438200 | 1.437730 | -0.03 | 1.00 | 4 | 7 | 0.25 0.10-0.11 0.03 0.66 0.07 |
| 52 | 1.440000 | 1.439525 | -0.03 | 1.00 | 3 | 7 | 0.52 0.70-0.53 0.08 0.15 0.09 |

Bulk Modulus= 2.187

| c11 | c22 | c33 | c23 | c13 | c12 | c44 | c55 | c66 |
|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| 3.9780 | 3.9780 | 4.6961 | 1.5295 | 1.5295 | 0.7394 | 1.0656 | 1.0656 | 0.4750 |

| d1 | d2 | d3 |
|---------|---------|---------|
| 0.46470 | 0.46400 | 0.31820 |

loop# 7 rms error= 0.3697 %, changed by -.0000005 %

length of gradient vector= 0.000000 blamb= 0.000586

| eigenvalues | eigenvectors |
|-------------|--------------------------------|
| 0.00179 | -0.36 0.46-0.63 0.50-0.12 0.06 |
| 0.02686 | -0.65-0.69 0.10 0.29-0.03 0.02 |
| 0.16526 | -0.56 0.16-0.21-0.78 0.09-0.05 |
| 0.53582 | -0.37 0.53 0.74 0.18 0.01 0.00 |
| 3.48856 | 0.01-0.02 0.06-0.15-0.97 0.16 |
| 15.51152 | 0.00 0.00 0.01-0.05 0.17 0.98 |

chisquare increased 2% by the following % changes in independent parameters

| | | | | | |
|-------|-------|-------|-------|-------|-------|
| -1.03 | -1.57 | -4.15 | -5.67 | 0.09 | 0.06 |
| 0.34 | -0.43 | 0.30 | 2.09 | -0.05 | -0.01 |
| -0.19 | 0.03 | -0.16 | 1.19 | 0.07 | 0.03 |

zircon 1172 K
 free moduli are c11, c33, c23, c12, c44, c66
 using 12 order polynomials mass= 0.3167 gm rho= 4.607 gm/cc

| n | fex | fr | %err | wt | k | i | df/d(moduli) |
|----|----------|----------|-------|------|---|---|-------------------------------|
| 1 | 0.302860 | 0.299950 | -0.96 | 1.00 | 4 | 1 | 0.00 0.00 0.00 0.00 0.17 0.82 |
| 2 | 0.436360 | 0.436372 | 0.00 | 1.00 | 3 | 2 | 0.02 0.00-0.01 0.00 0.00 0.98 |
| 3 | 0.586140 | 0.588499 | 0.40 | 1.00 | 7 | 2 | 0.33 0.05-0.09 0.00 0.00 0.71 |
| 4 | 0.592760 | 0.589985 | -0.47 | 1.00 | 1 | 2 | 0.33 0.05-0.09 0.00 0.00 0.71 |
| 5 | 0.653150 | 0.653713 | 0.09 | 1.00 | 6 | 2 | 0.85 0.01-0.02-0.13 0.30 0.00 |
| 6 | 0.673630 | 0.671416 | -0.33 | 1.00 | 4 | 2 | 0.05 0.00 0.00-0.01 0.95 0.01 |
| 7 | 0.676480 | 0.677031 | 0.08 | 1.00 | 6 | 3 | 0.72 0.15-0.30 0.09 0.33 0.00 |
| 8 | 0.737840 | 0.740392 | 0.35 | 1.00 | 8 | 2 | 0.40 0.04-0.07-0.02 0.34 0.32 |
| 9 | 0.748190 | 0.741757 | -0.86 | 1.00 | 2 | 2 | 0.40 0.04-0.07-0.02 0.34 0.32 |
| 10 | 0.791480 | 0.793418 | 0.24 | 1.00 | 2 | 3 | 0.07 0.01-0.01 0.00 0.93 0.01 |
| 11 | 0.792970 | 0.794041 | 0.13 | 1.00 | 8 | 3 | 0.07 0.01-0.01 0.00 0.93 0.01 |
| 12 | 0.895650 | 0.894962 | -0.08 | 1.00 | 5 | 1 | 1.23 0.01-0.01-0.23 0.00 0.00 |
| 13 | 0.897930 | 0.898760 | 0.09 | 1.00 | 5 | 2 | 1.11 0.29-0.39-0.01 0.00 0.00 |
| 14 | 0.900460 | 0.901683 | 0.14 | 1.00 | 5 | 3 | 1.03 0.49-0.67 0.15 0.00 0.00 |
| 15 | 0.911710 | 0.912132 | 0.05 | 1.00 | 3 | 3 | 0.15 0.02-0.03 0.00 0.00 0.86 |
| 16 | 0.912860 | 0.915666 | 0.31 | 1.00 | 8 | 4 | 0.35 0.05-0.09 0.00 0.54 0.15 |
| 17 | 0.926250 | 0.916563 | -1.05 | 1.00 | 2 | 4 | 0.35 0.05-0.09 0.00 0.54 0.16 |
| 18 | 0.955310 | 0.955982 | 0.07 | 1.00 | 7 | 3 | 0.83 0.29-0.34 0.00 0.01 0.21 |
| 19 | 0.958290 | 0.957199 | -0.11 | 1.00 | 1 | 3 | 0.83 0.29-0.34 0.00 0.01 0.21 |
| 20 | 0.968930 | 0.970175 | 0.13 | 1.00 | 4 | 3 | 0.07 0.01-0.02 0.01 0.82 0.11 |
| 21 | 1.023000 | 1.021810 | -0.12 | 1.00 | 6 | 4 | 0.43 0.06-0.11 0.00 0.33 0.29 |
| 22 | 1.027700 | 1.031695 | 0.39 | 1.00 | 3 | 4 | 0.08 0.03-0.04 0.00 0.00 0.92 |
| 23 | 1.117800 | 1.119198 | 0.13 | 1.00 | 4 | 4 | 0.10 0.02-0.02-0.01 0.38 0.53 |
| 24 | 1.138100 | 1.129154 | -0.79 | 1.00 | 6 | 5 | 0.76 0.11-0.18-0.02 0.34 0.00 |
| 25 | 1.145100 | 1.145200 | 0.01 | 1.00 | 5 | 4 | 0.59 0.55-0.44 0.04 0.02 0.24 |
| 26 | 1.168200 | 1.167933 | -0.02 | 1.00 | 3 | 5 | 0.19 0.82-0.38 0.03 0.23 0.11 |
| 27 | 1.175600 | 1.174175 | -0.12 | 1.00 | 1 | 4 | 0.54 0.38-0.23-0.03 0.19 0.15 |
| 28 | 0.000000 | 1.174229 | 0.00 | 0.00 | 7 | 4 | 0.54 0.38-0.23-0.03 0.19 0.15 |
| 29 | 1.186800 | 1.187154 | 0.03 | 1.00 | 4 | 5 | 0.04 0.01-0.01 0.00 0.34 0.63 |
| 30 | 0.000000 | 1.228067 | 0.00 | 0.00 | 7 | 5 | 0.33 0.74-0.38 0.04 0.18 0.09 |
| 31 | 1.234000 | 1.228401 | -0.45 | 1.00 | 1 | 5 | 0.33 0.74-0.38 0.04 0.18 0.09 |
| 32 | 0.000000 | 1.243185 | 0.00 | 0.00 | 5 | 5 | 0.52 0.56-0.14-0.07 0.13 0.00 |
| 33 | 1.243100 | 1.246210 | 0.25 | 1.00 | 6 | 6 | 0.42 0.04-0.03-0.07 0.63 0.00 |
| 34 | 1.248700 | 1.254042 | 0.43 | 1.00 | 7 | 6 | 0.30 0.21-0.06-0.02 0.14 0.44 |
| 35 | 1.258400 | 1.255183 | -0.26 | 1.00 | 1 | 6 | 0.30 0.21-0.06-0.02 0.14 0.43 |
| 36 | 1.263900 | 1.262606 | -0.10 | 1.00 | 6 | 7 | 0.41 0.17-0.24 0.06 0.59 0.00 |
| 37 | 1.281800 | 1.279658 | -0.17 | 1.00 | 3 | 6 | 0.28 0.35-0.20-0.01 0.52 0.06 |
| 38 | 1.302500 | 1.303787 | 0.10 | 1.00 | 2 | 5 | 0.36 0.08-0.07-0.04 0.57 0.10 |
| 39 | 1.303600 | 1.305728 | 0.16 | 1.00 | 8 | 5 | 0.36 0.08-0.07-0.04 0.56 0.11 |
| 40 | 0.000000 | 1.312816 | 0.00 | 0.00 | 5 | 6 | 0.46 0.51-0.26 0.02 0.09 0.17 |
| 41 | 1.330600 | 1.333710 | 0.23 | 1.00 | 8 | 6 | 0.31 0.08-0.09-0.01 0.62 0.09 |
| 42 | 1.332800 | 1.334831 | 0.15 | 1.00 | 2 | 6 | 0.31 0.08-0.09-0.01 0.62 0.09 |
| 43 | 1.335900 | 1.335224 | -0.05 | 1.00 | 5 | 7 | 0.49 0.49-0.26 0.01 0.04 0.22 |
| 44 | 1.357000 | 1.363789 | 0.50 | 1.00 | 2 | 7 | 0.37 0.05-0.10 0.02 0.44 0.22 |
| 45 | 1.364400 | 1.364935 | 0.04 | 1.00 | 8 | 7 | 0.37 0.05-0.10 0.02 0.44 0.21 |
| 46 | 1.367300 | 1.374416 | 0.52 | 1.00 | 7 | 7 | 0.30 0.16-0.13 0.00 0.04 0.63 |
| 47 | 1.374100 | 1.375580 | 0.11 | 1.00 | 1 | 7 | 0.30 0.17-0.13 0.00 0.04 0.63 |
| 48 | 1.404500 | 1.408451 | 0.28 | 1.00 | 4 | 6 | 0.32 0.03-0.01-0.04 0.67 0.03 |
| 49 | 1.418000 | 1.422695 | 0.33 | 1.00 | 1 | 8 | 0.54 0.52-0.30-0.02 0.14 0.12 |
| 50 | 1.420100 | 1.423278 | 0.22 | 1.00 | 7 | 8 | 0.52 0.51-0.30-0.02 0.16 0.12 |
| 51 | 1.429600 | 1.429884 | 0.02 | 1.00 | 3 | 7 | 0.52 0.70-0.54 0.08 0.15 0.09 |
| 52 | 1.431700 | 1.430123 | -0.11 | 1.00 | 4 | 7 | 0.25 0.10-0.11 0.03 0.66 0.07 |

Bulk Modulus= 2.166

| c11 | c22 | c33 | c23 | c13 | c12 | c44 | c55 | c66 |
|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| 3.9282 | 3.9282 | 4.6389 | 1.5208 | 1.5208 | 0.7409 | 1.0542 | 1.0542 | 0.4720 |

| d1 | d2 | d3 |
|---------|---------|---------|
| 0.46510 | 0.46420 | 0.31840 |

loop# 7 rms error= 0.3579 %, changed by -.0000012 %

length of gradient vector= 0.000001 blamb= 0.000890

| eigenvalues | eigenvectors |
|-------------|--------------------------------|
| 0.00198 | -0.36 0.47-0.59 0.53-0.13 0.06 |
| 0.03259 | -0.65-0.69 0.13 0.29-0.04 0.02 |
| 0.17897 | -0.56 0.15-0.26-0.77 0.11-0.06 |
| 0.65857 | -0.37 0.53 0.75 0.12 0.01 0.00 |
| 3.69325 | 0.01-0.01 0.05-0.17-0.97 0.17 |
| 15.78038 | 0.00 0.00 0.01-0.06 0.18 0.98 |

chisquare increased 2% by the following % changes in independent parameters

| | | | | | |
|-------|-------|-------|-------|-------|-------|
| -1.01 | -1.53 | -4.00 | -5.43 | 0.09 | 0.06 |
| 0.32 | -0.40 | 0.26 | 1.94 | -0.03 | -0.01 |
| -0.17 | 0.03 | -0.20 | 1.16 | 0.06 | 0.03 |