*Supplementary Informations*

# Rationalization of lattice thermal expansion for beta-blocker organic crystals

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**Abstract:** Anisotropic lattice expansion could be source of misunderstanding in powder pattern recognitions especially in the case of organic crystals where for the interpretation of room temperature patterns single crystal data at low temperature are usually used. Trying to rationalize the thermal lattice expansion, we studied two close related β-blocker molecules with similar packing in the solid state but with different thermal behavior. Solid state calculations, using the fast and accurate HF-3c method and the quasi harmonic approximation for the simulation of the lattice expansion, were able to reproduce with good accuracy the experimental trends. The complete analysis of the calculated thermal expansion of the two structures as well as of other structures with similar packing found in a database survey, revealed the primary role of the hydrogen bonds. Secondary non covalent interactions in the plane perpendicular to the hydrogen bond system could also have a role.

**Keywords:** Anisotropic thermal expansion; solid state calculations; organic crystals; Quasi Harmonic Approximation; β-blocker molecules

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Optimized coordinates and thermal properties calculated using Quasi Harmonic Approsimation of Metoprolol, Betaxolol I, POLMET, KAZPOQ, PROPRA10 and IMITON.

**Metoprolol**

Optimized Geometry:

SPACE GROUP (CENTROSYMMETRIC) : P 21/C

15.919843 5.212660 21.401479 90.000 125.145 90.000

O 0.280908 0.076146 -0.310721
O 0.062041 0.226240 -0.429663
H 0.032370 0.065212 -0.425262
O -0.350717 -0.462117 0.032822
N 0.007837 0.247083 0.421356

| | | | |
|---|---|---|---|
| H | -0.035765 | 0.374980 | 0.426998 |
| C | 0.375538 | 0.110958 | -0.244041 |
| C | 0.439527 | 0.317832 | -0.229577 |
| H | 0.417179 | 0.465459 | -0.271627 |
| C | -0.465335 | 0.334589 | -0.159550 |
| H | -0.416857 | 0.496508 | -0.149017 |
| C | -0.432287 | 0.149146 | -0.103982 |
| C | -0.496521 | -0.058927 | -0.119226 |
| H | -0.470318 | -0.207008 | -0.076369 |
| C | 0.408632 | -0.078694 | -0.187947 |
| H | 0.358902 | -0.239823 | -0.200119 |
| C | 0.246946 | 0.252687 | -0.371327 |
| H | 0.240570 | 0.447183 | -0.355040 |
| H | 0.300680 | 0.259881 | -0.387596 |
| C | 0.138889 | 0.161758 | -0.440646 |
| H | 0.142906 | -0.045993 | -0.445786 |
| C | 0.115772 | 0.288676 | 0.484855 |
| H | 0.133777 | 0.492578 | 0.494735 |
| H | 0.165702 | 0.202872 | 0.471344 |
| C | -0.012013 | 0.278063 | 0.345377 |
| H | 0.029770 | 0.442897 | 0.345012 |
| C | 0.023227 | 0.035543 | 0.324393 |
| H | 0.103873 | -0.003708 | 0.366852 |
| H | -0.021228 | -0.128812 | 0.320472 |
| H | 0.011455 | 0.062872 | 0.269750 |
| C | -0.128479 | 0.323320 | 0.285722 |
| H | -0.151050 | -0.495517 | 0.296878 |
| H | -0.146213 | 0.327735 | 0.228748 |
| H | -0.171982 | 0.169950 | 0.288975 |
| C | -0.329017 | 0.167005 | -0.026841 |
| H | -0.295403 | -0.022957 | -0.009949 |
| H | -0.277102 | 0.291063 | -0.030167 |
| C | -0.339103 | 0.266889 | 0.037047 |
| H | -0.405439 | 0.175543 | 0.030733 |
| H | -0.270758 | 0.210936 | 0.092937 |
| C | -0.362781 | -0.369113 | 0.089803 |
| H | -0.432325 | -0.445398 | 0.082111 |
| H | -0.369067 | -0.161120 | 0.085533 |
| H | -0.296889 | -0.419038 | 0.147463 |

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THERMAL PROPERTIES FROM HELMHOLTZ FREE ENERGY

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| T (K) | V (Ang^3) | Bt (GPa) | ALPHA (1/K) | Cp-Cv (J/mol*K) | Bs (GPa) | Sp-Sv (J/mol*K) |
|---|---|---|---|---|---|---|

| | | | | | | |
|---|---|---|---|---|---|---|
| 10.00 | 1497.0742 | 9.963 | 0.40425E-05 | 0.001 | 9.964 | 1.482 |
| 15.92 | 1497.0831 | 9.979 | 0.40424E-05 | 0.002 | 9.979 | 4.678 |
| 21.84 | 1497.1458 | 9.995 | 0.10106E-04 | 0.020 | 9.997 | 8.245 |
| 27.76 | 1497.2622 | 10.013 | 0.16252E-04 | 0.066 | 10.018 | 11.653 |
| 33.67 | 1497.4323 | 10.034 | 0.21891E-04 | 0.146 | 10.042 | 14.729 |
| 39.59 | 1497.6472 | 10.059 | 0.26350E-04 | 0.249 | 10.070 | 17.435 |
| 45.51 | 1497.8980 | 10.089 | 0.30386E-04 | 0.382 | 10.103 | 19.791 |
| 51.43 | 1498.1845 | 10.122 | 0.33915E-04 | 0.540 | 10.140 | 21.841 |
| 57.35 | 1498.4979 | 10.157 | 0.36852E-04 | 0.714 | 10.179 | 23.632 |
| 63.27 | 1498.8382 | 10.195 | 0.40041E-04 | 0.933 | 10.220 | 25.210 |
| 69.18 | 1499.2053 | 10.233 | 0.41965E-04 | 1.126 | 10.261 | 26.612 |
| 75.10 | 1499.5814 | 10.274 | 0.43384E-04 | 1.311 | 10.304 | 27.865 |
| 81.02 | 1499.9754 | 10.315 | 0.44885E-04 | 1.521 | 10.348 | 28.998 |
| 86.94 | 1500.3783 | 10.356 | 0.46470E-04 | 1.757 | 10.393 | 30.028 |
| 92.86 | 1500.7991 | 10.397 | 0.47368E-04 | 1.958 | 10.436 | 30.975 |
| 98.78 | 1501.2200 | 10.439 | 0.48369E-04 | 2.181 | 10.480 | 31.845 |
| 104.69 | 1501.6588 | 10.479 | 0.49162E-04 | 2.398 | 10.523 | 32.656 |
| 110.61 | 1502.0975 | 10.520 | 0.49862E-04 | 2.617 | 10.566 | 33.410 |
| 116.53 | 1502.5452 | 10.560 | 0.50348E-04 | 2.822 | 10.607 | 34.118 |
| 122.45 | 1502.9929 | 10.599 | 0.50840E-04 | 3.036 | 10.649 | 34.783 |
| 128.37 | 1503.4496 | 10.637 | 0.51130E-04 | 3.232 | 10.688 | 35.413 |
| 134.29 | 1503.9063 | 10.674 | 0.51322E-04 | 3.419 | 10.727 | 36.008 |
| 140.20 | 1504.3630 | 10.712 | 0.51501E-04 | 3.609 | 10.766 | 36.573 |
| 146.12 | 1504.8196 | 10.748 | 0.51589E-04 | 3.788 | 10.803 | 37.111 |
| 152.04 | 1505.2852 | 10.782 | 0.51775E-04 | 3.983 | 10.839 | 37.628 |
| 157.96 | 1505.7419 | 10.817 | 0.51765E-04 | 4.151 | 10.875 | 38.120 |
| 163.88 | 1506.2075 | 10.849 | 0.51743E-04 | 4.318 | 10.908 | 38.595 |
| 169.80 | 1506.6642 | 10.881 | 0.51733E-04 | 4.487 | 10.941 | 39.048 |
| 175.71 | 1507.1298 | 10.911 | 0.51517E-04 | 4.618 | 10.972 | 39.488 |
| 181.63 | 1507.5865 | 10.942 | 0.51598E-04 | 4.804 | 11.004 | 39.911 |
| 187.55 | 1508.0432 | 10.971 | 0.51284E-04 | 4.915 | 11.033 | 40.319 |
| 193.47 | 1508.5088 | 10.997 | 0.51171E-04 | 5.061 | 11.060 | 40.718 |
| 199.39 | 1508.9565 | 11.025 | 0.51052E-04 | 5.206 | 11.089 | 41.099 |
| 205.31 | 1509.4132 | 11.050 | 0.50733E-04 | 5.308 | 11.114 | 41.473 |
| 211.22 | 1509.8698 | 11.074 | 0.50821E-04 | 5.493 | 11.139 | 41.837 |
| 217.14 | 1510.3176 | 11.098 | 0.50605E-04 | 5.613 | 11.163 | 42.189 |
| 223.06 | 1510.7742 | 11.119 | 0.50195E-04 | 5.685 | 11.183 | 42.536 |
| 228.98 | 1511.2219 | 11.140 | 0.49979E-04 | 5.799 | 11.204 | 42.871 |
| 234.90 | 1511.6607 | 11.161 | 0.49558E-04 | 5.861 | 11.225 | 43.197 |
| 240.82 | 1512.1084 | 11.178 | 0.49343E-04 | 5.968 | 11.243 | 43.518 |
| 246.73 | 1512.5472 | 11.196 | 0.49231E-04 | 6.099 | 11.261 | 43.831 |
| 252.65 | 1512.9859 | 11.213 | 0.49012E-04 | 6.201 | 11.278 | 44.137 |
| 258.57 | 1513.4247 | 11.228 | 0.48997E-04 | 6.352 | 11.293 | 44.438 |
| 264.49 | 1513.8635 | 11.241 | 0.48788E-04 | 6.452 | 11.306 | 44.734 |
| 270.41 | 1514.3022 | 11.253 | 0.48476E-04 | 6.521 | 11.318 | 45.025 |
| 276.33 | 1514.7320 | 11.264 | 0.48160E-04 | 6.585 | 11.329 | 45.308 |
| 282.24 | 1515.1618 | 11.274 | 0.47747E-04 | 6.619 | 11.338 | 45.586 |
| 288.16 | 1515.5916 | 11.283 | 0.47630E-04 | 6.732 | 11.347 | 45.861 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 294.08 | 1516.0125 | 11.291 | 0.47504E-04 | 6.841 | 11.355 | 46.128 |
| 300.00 | 1516.4423 | 11.296 | 0.47391E-04 | 6.951 | 11.360 | 46.395 |

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LINEAR THERMAL EXPANSION OF CONVENTIONAL LATTICE PARAMETERS

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| T (K) | a (Ang) | ALPHA_a (1/K) | b (Ang) | ALPHA_b (1/K) | c (Ang) | ALPHA_c (1/K) |
|---|---|---|---|---|---|---|
| 10.00 | 16.2368 | 0.39320E-05 | 5.2503 | 0.11393E-07 | 21.6807 | 0.21933E-05 |
| 15.92 | 16.2369 | 0.39331E-05 | 5.2503 | 0.10573E-07 | 21.6808 | 0.21936E-05 |
| 21.84 | 16.2376 | 0.98367E-05 | 5.2503 | 0.23281E-07 | 21.6813 | 0.54853E-05 |
| 27.76 | 16.2388 | 0.15858E-04 | 5.2503 | 0.97173E-08 | 21.6822 | 0.88339E-05 |
| 33.67 | 16.2406 | 0.21436E-04 | 5.2503 | -0.40286E-07 | 21.6835 | 0.11923E-04 |
| 39.59 | 16.2429 | 0.25915E-04 | 5.2503 | -0.12984E-06 | 21.6852 | 0.14389E-04 |
| 45.51 | 16.2456 | 0.30041E-04 | 5.2503 | -0.26195E-06 | 21.6872 | 0.16643E-04 |
| 51.43 | 16.2486 | 0.33727E-04 | 5.2503 | -0.43309E-06 | 21.6895 | 0.18639E-04 |
| 57.35 | 16.2520 | 0.36887E-04 | 5.2502 | -0.64132E-06 | 21.6920 | 0.20330E-04 |
| 63.27 | 16.2557 | 0.40363E-04 | 5.2502 | -0.90046E-06 | 21.6947 | 0.22180E-04 |
| 69.18 | 16.2598 | 0.42617E-04 | 5.2502 | -0.11687E-05 | 21.6976 | 0.23346E-04 |
| 75.10 | 16.2639 | 0.44406E-04 | 5.2501 | -0.14579E-05 | 21.7007 | 0.24247E-04 |
| 81.02 | 16.2683 | 0.46311E-04 | 5.2501 | -0.17717E-05 | 21.7039 | 0.25203E-04 |
| 86.94 | 16.2728 | 0.48351E-04 | 5.2500 | -0.21247E-05 | 21.7072 | 0.26222E-04 |
| 92.86 | 16.2776 | 0.49716E-04 | 5.2500 | -0.24740E-05 | 21.7106 | 0.26866E-04 |
| 98.78 | 16.2824 | 0.51207E-04 | 5.2499 | -0.28422E-05 | 21.7141 | 0.27573E-04 |
| 104.69 | 16.2875 | 0.52509E-04 | 5.2498 | -0.32207E-05 | 21.7177 | 0.28171E-04 |
| 110.61 | 16.2926 | 0.53732E-04 | 5.2497 | -0.36080E-05 | 21.7213 | 0.28723E-04 |
| 116.53 | 16.2978 | 0.54752E-04 | 5.2496 | -0.39993E-05 | 21.7251 | 0.29159E-04 |
| 122.45 | 16.3031 | 0.55794E-04 | 5.2494 | -0.44022E-05 | 21.7288 | 0.29603E-04 |
| 128.37 | 16.3086 | 0.56629E-04 | 5.2493 | -0.47992E-05 | 21.7327 | 0.29935E-04 |
| 134.29 | 16.3141 | 0.57366E-04 | 5.2491 | -0.51942E-05 | 21.7366 | 0.30212E-04 |
| 140.20 | 16.3197 | 0.58106E-04 | 5.2490 | -0.55997E-05 | 21.7405 | 0.30486E-04 |
| 146.12 | 16.3253 | 0.58745E-04 | 5.2488 | -0.59982E-05 | 21.7444 | 0.30708E-04 |
| 152.04 | 16.3311 | 0.59506E-04 | 5.2486 | -0.64154E-05 | 21.7484 | 0.30989E-04 |
| 157.96 | 16.3368 | 0.60045E-04 | 5.2484 | -0.68114E-05 | 21.7524 | 0.31155E-04 |
| 163.88 | 16.3427 | 0.60582E-04 | 5.2482 | -0.72134E-05 | 21.7564 | 0.31317E-04 |
| 169.80 | 16.3485 | 0.61129E-04 | 5.2479 | -0.76152E-05 | 21.7604 | 0.31485E-04 |
| 175.71 | 16.3545 | 0.61435E-04 | 5.2477 | -0.79896E-05 | 21.7645 | 0.31527E-04 |
| 181.63 | 16.3605 | 0.62101E-04 | 5.2474 | -0.84130E-05 | 21.7686 | 0.31753E-04 |
| 187.55 | 16.3665 | 0.62288E-04 | 5.2472 | -0.87702E-05 | 21.7726 | 0.31735E-04 |
| 193.47 | 16.3726 | 0.62716E-04 | 5.2469 | -0.91596E-05 | 21.7768 | 0.31840E-04 |
| 199.39 | 16.3786 | 0.63140E-04 | 5.2466 | -0.95508E-05 | 21.7808 | 0.31941E-04 |
| 205.31 | 16.3848 | 0.63313E-04 | 5.2463 | -0.99027E-05 | 21.7850 | 0.31917E-04 |
| 211.22 | 16.3910 | 0.63990E-04 | 5.2460 | -0.10332E-04 | 21.7891 | 0.32147E-04 |
| 217.14 | 16.3971 | 0.64289E-04 | 5.2457 | -0.10702E-04 | 21.7932 | 0.32185E-04 |
| 223.06 | 16.4035 | 0.64331E-04 | 5.2453 | -0.11024E-04 | 21.7974 | 0.32097E-04 |
| 228.98 | 16.4097 | 0.64618E-04 | 5.2450 | -0.11386E-04 | 21.8016 | 0.32132E-04 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 234.90 | 16.4159 | 0.64637E-04 | 5.2446 | -0.11700E-04 | 21.8057 | 0.32034E-04 |
| 240.82 | 16.4223 | 0.64914E-04 | 5.2442 | -0.12055E-04 | 21.8098 | 0.32065E-04 |
| 246.73 | 16.4286 | 0.65322E-04 | 5.2439 | -0.12432E-04 | 21.8140 | 0.32162E-04 |
| 252.65 | 16.4349 | 0.65591E-04 | 5.2435 | -0.12785E-04 | 21.8181 | 0.32190E-04 |
| 258.57 | 16.4413 | 0.66130E-04 | 5.2431 | -0.13190E-04 | 21.8223 | 0.32351E-04 |
| 264.49 | 16.4478 | 0.66403E-04 | 5.2427 | -0.13539E-04 | 21.8265 | 0.32381E-04 |
| 270.41 | 16.4543 | 0.66532E-04 | 5.2422 | -0.13857E-04 | 21.8307 | 0.32343E-04 |
| 276.33 | 16.4607 | 0.66651E-04 | 5.2418 | -0.14172E-04 | 21.8348 | 0.32300E-04 |
| 282.24 | 16.4672 | 0.66625E-04 | 5.2414 | -0.14450E-04 | 21.8390 | 0.32188E-04 |
| 288.16 | 16.4738 | 0.67009E-04 | 5.2409 | -0.14815E-04 | 21.8432 | 0.32276E-04 |
| 294.08 | 16.4802 | 0.67388E-04 | 5.2404 | -0.15184E-04 | 21.8473 | 0.32359E-04 |
| 300.00 | 16.4869 | 0.67220E-04 | 5.2400 | -0.15154E-04 | 21.8515 | 0.32285E-04 |

**Betaxolol I**

Optimized Geometry:

SPACE GROUP (CENTROSYMMETRIC) : P -1

4.759211 9.639602 18.658671 104.181 93.534 100.977

| | | | |
|---|---|---|---|
| O | -0.499536 | -0.332002 | 0.332820 |
| O | 0.292915 | -0.000212 | 0.424230 |
| H | 0.478141 | 0.070109 | 0.435487 |
| O | -0.103467 | 0.232853 | -0.031725 |
| N | 0.166998 | -0.162371 | -0.468063 |
| H | 0.036189 | -0.087977 | -0.460979 |
| C | 0.387974 | -0.209207 | 0.334849 |
| H | 0.177499 | -0.236552 | 0.301989 |
| H | -0.471594 | -0.129616 | 0.313142 |
| C | 0.365801 | -0.133902 | 0.417275 |
| H | -0.421927 | -0.121737 | 0.446649 |
| C | 0.153258 | -0.232264 | 0.452359 |
| H | -0.062615 | -0.254151 | 0.423523 |
| H | 0.218607 | -0.336091 | 0.445238 |
| C | 0.067885 | -0.263729 | -0.423529 |
| H | 0.217539 | -0.336073 | -0.424926 |
| C | 0.077985 | -0.173838 | -0.343260 |
| H | 0.295163 | -0.114453 | -0.322091 |
| H | 0.006881 | -0.244714 | -0.308373 |
| H | -0.060095 | -0.096189 | -0.340896 |
| C | -0.232404 | -0.358939 | -0.452444 |
| H | -0.382024 | -0.291222 | -0.459534 |
| H | -0.306583 | -0.420695 | -0.413598 |
| H | -0.229983 | -0.434770 | 0.494581 |
| C | -0.382558 | -0.386614 | 0.271644 |
| C | -0.240451 | -0.498301 | 0.274877 |
| H | -0.235522 | 0.465226 | 0.324936 |

| | | | |
|---|---|---|---|
| C | -0.108339 | 0.440637 | 0.216148 |
| H | 0.001948 | 0.354262 | 0.219432 |
| C | -0.111553 | 0.488013 | 0.152303 |
| C | -0.387846 | -0.339811 | 0.207577 |
| H | -0.498153 | -0.254902 | 0.202540 |
| C | -0.252720 | -0.402182 | 0.149105 |
| H | -0.256259 | -0.363282 | 0.099639 |
| C | 0.020526 | 0.414550 | 0.085515 |
| H | 0.126994 | 0.494903 | 0.058999 |
| H | 0.179045 | 0.358289 | 0.102330 |
| C | -0.217867 | 0.303519 | 0.029690 |
| H | -0.328358 | 0.225811 | 0.058035 |
| H | -0.379576 | 0.360872 | 0.013900 |
| C | -0.315669 | 0.122806 | -0.077429 |
| H | 0.497761 | 0.165189 | -0.092384 |
| H | -0.395248 | 0.038790 | -0.049054 |
| C | -0.199478 | 0.050658 | -0.147855 |
| H | -0.153608 | 0.119004 | -0.185326 |
| C | -0.007005 | -0.052855 | -0.144745 |
| H | 0.043229 | -0.074048 | -0.092017 |
| H | 0.166255 | -0.052712 | -0.178943 |
| C | -0.306215 | -0.109208 | -0.181839 |
| H | -0.339572 | -0.148355 | -0.241395 |
| H | -0.458743 | -0.169215 | -0.154424 |

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THERMAL PROPERTIES FROM HELMHOLTZ FREE ENERGY

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| T (K) | V (Ang^3) | Bt (GPa) | ALPHA (1/K) | Cp-Cv (J/mol*K) | Bs (GPa) | Sp-Sv (J/mol*K) |
|---|---|---|---|---|---|---|
| 10.00 | 846.3238 | 11.102 | 0.16150E-04 | 0.015 | 11.136 | 0.987 |
| 15.92 | 846.3777 | 11.088 | 0.16283E-04 | 0.024 | 11.102 | 3.266 |
| 21.84 | 846.4855 | 11.062 | 0.28032E-04 | 0.097 | 11.089 | 6.167 |
| 27.76 | 846.6608 | 11.023 | 0.41928E-04 | 0.274 | 11.072 | 9.201 |
| 33.67 | 846.9035 | 10.975 | 0.54020E-04 | 0.550 | 11.046 | 12.128 |
| 39.59 | 847.2001 | 10.921 | 0.64756E-04 | 0.925 | 11.014 | 14.857 |
| 45.51 | 847.5506 | 10.861 | 0.74025E-04 | 1.382 | 10.976 | 17.368 |
| 51.43 | 847.9416 | 10.798 | 0.82833E-04 | 1.946 | 10.937 | 19.668 |
| 57.35 | 848.3798 | 10.731 | 0.90063E-04 | 2.550 | 10.891 | 21.783 |
| 63.27 | 848.8449 | 10.663 | 0.96611E-04 | 3.219 | 10.843 | 23.727 |
| 69.18 | 849.3505 | 10.592 | 0.10359E-03 | 4.022 | 10.796 | 25.534 |
| 75.10 | 849.8830 | 10.520 | 0.10777E-03 | 4.697 | 10.738 | 27.218 |
| 81.02 | 850.4358 | 10.447 | 0.11328E-03 | 5.563 | 10.686 | 28.794 |
| 86.94 | 851.0222 | 10.372 | 0.11789E-03 | 6.423 | 10.629 | 30.290 |
| 92.86 | 851.6222 | 10.297 | 0.12166E-03 | 7.258 | 10.569 | 31.705 |
| 98.78 | 852.2491 | 10.220 | 0.12557E-03 | 8.170 | 10.509 | 33.061 |
| 104.69 | 852.8895 | 10.143 | 0.12923E-03 | 9.110 | 10.448 | 34.360 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 110.61 | 853.5568 | 10.065 | 0.13247E-03 | 10.043 | 10.384 | 35.620 |
| 116.53 | 854.2309 | 9.987 | 0.13584E-03 | 11.047 | 10.321 | 36.834 |
| 122.45 | 854.9252 | 9.908 | 0.13866E-03 | 12.009 | 10.254 | 38.018 |
| 128.37 | 855.6398 | 9.827 | 0.14175E-03 | 13.061 | 10.188 | 39.178 |
| 134.29 | 856.3611 | 9.747 | 0.14456E-03 | 14.106 | 10.120 | 40.309 |
| 140.20 | 857.1026 | 9.666 | 0.14722E-03 | 15.161 | 10.051 | 41.425 |
| 146.12 | 857.8576 | 9.584 | 0.14994E-03 | 16.265 | 9.981 | 42.524 |
| 152.04 | 858.6260 | 9.501 | 0.15230E-03 | 17.327 | 9.909 | 43.610 |
| 157.96 | 859.4059 | 9.418 | 0.15466E-03 | 18.418 | 9.836 | 44.684 |
| 163.88 | 860.1984 | 9.334 | 0.15709E-03 | 19.554 | 9.762 | 45.748 |
| 169.80 | 861.0049 | 9.249 | 0.15964E-03 | 20.753 | 9.688 | 46.808 |
| 175.71 | 861.8255 | 9.163 | 0.16198E-03 | 21.924 | 9.612 | 47.864 |
| 181.63 | 862.6601 | 9.076 | 0.16443E-03 | 23.155 | 9.534 | 48.918 |
| 187.55 | 863.5017 | 8.989 | 0.16674E-03 | 24.374 | 9.456 | 49.965 |
| 193.47 | 864.3643 | 8.900 | 0.16904E-03 | 25.612 | 9.375 | 51.020 |
| 199.39 | 865.2340 | 8.811 | 0.17148E-03 | 26.916 | 9.294 | 52.070 |
| 205.31 | 866.1177 | 8.720 | 0.17376E-03 | 28.193 | 9.210 | 53.124 |
| 211.22 | 867.0154 | 8.628 | 0.17631E-03 | 29.580 | 9.126 | 54.182 |
| 217.14 | 867.9271 | 8.535 | 0.17886E-03 | 30.988 | 9.041 | 55.245 |
| 223.06 | 868.8529 | 8.440 | 0.18140E-03 | 32.414 | 8.953 | 56.314 |
| 228.98 | 869.7927 | 8.344 | 0.18393E-03 | 33.854 | 8.863 | 57.390 |
| 234.90 | 870.7465 | 8.246 | 0.18645E-03 | 35.309 | 8.770 | 58.473 |
| 240.82 | 871.7143 | 8.147 | 0.18922E-03 | 36.876 | 8.677 | 59.563 |
| 246.73 | 872.6962 | 8.046 | 0.19213E-03 | 38.512 | 8.582 | 60.662 |
| 252.65 | 873.6991 | 7.942 | 0.19503E-03 | 40.159 | 8.484 | 61.776 |
| 258.57 | 874.7161 | 7.836 | 0.19806E-03 | 41.869 | 8.383 | 62.899 |
| 264.49 | 875.7470 | 7.728 | 0.20094E-03 | 43.525 | 8.279 | 64.032 |
| 270.41 | 876.7990 | 7.618 | 0.20433E-03 | 45.413 | 8.173 | 65.181 |
| 276.33 | 877.8651 | 7.505 | 0.20787E-03 | 47.370 | 8.065 | 66.341 |
| 282.24 | 878.9592 | 7.388 | 0.21138E-03 | 49.317 | 7.952 | 67.524 |
| 288.16 | 880.0673 | 7.268 | 0.21529E-03 | 51.447 | 7.837 | 68.718 |
| 294.08 | 881.1964 | 7.145 | 0.21927E-03 | 53.607 | 7.717 | 69.929 |
| 300.00 | 882.3536 | 7.017 | 0.21891E-03 | 53.603 | 7.569 | 71.166 |

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LINEAR THERMAL EXPANSION OF CONVENTIONAL LATTICE PARAMETERS

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| T (K) | a (Ang) | ALPHA_a (1/K) | b (Ang) | ALPHA_b (1/K) | c (Ang) | ALPHA_c (1/K) |
|---|---|---|---|---|---|---|
| 10.00 | 4.8626 | 0.49586E-05 | 9.6063 | 0.27704E-05 | 19.0185 | 0.72784E-05 |
| 15.92 | 4.8627 | 0.50001E-05 | 9.6064 | 0.27947E-05 | 19.0191 | 0.73377E-05 |
| 21.84 | 4.8629 | 0.86110E-05 | 9.6066 | 0.48236E-05 | 19.0201 | 0.12622E-04 |
| 27.76 | 4.8632 | 0.12890E-04 | 9.6070 | 0.72617E-05 | 19.0219 | 0.18840E-04 |
| 33.67 | 4.8637 | 0.16627E-04 | 9.6074 | 0.94384E-05 | 19.0244 | 0.24206E-04 |
| 39.59 | 4.8642 | 0.19960E-04 | 9.6080 | 0.11441E-04 | 19.0273 | 0.28912E-04 |
| 45.51 | 4.8648 | 0.22856E-04 | 9.6087 | 0.13246E-04 | 19.0308 | 0.32910E-04 |

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|---|---|---|---|---|---|---|
| 51.43 | 4.8655 | 0.25627E-04 | 9.6095 | 0.15044E-04 | 19.0347 | 0.36642E-04 |
| 57.35 | 4.8663 | 0.27926E-04 | 9.6104 | 0.16620E-04 | 19.0391 | 0.39622E-04 |
| 63.27 | 4.8671 | 0.30031E-04 | 9.6114 | 0.18148E-04 | 19.0437 | 0.42236E-04 |
| 69.18 | 4.8680 | 0.32289E-04 | 9.6125 | 0.19828E-04 | 19.0486 | 0.44982E-04 |
| 75.10 | 4.8690 | 0.33691E-04 | 9.6137 | 0.21043E-04 | 19.0538 | 0.46450E-04 |
| 81.02 | 4.8700 | 0.35528E-04 | 9.6149 | 0.22592E-04 | 19.0591 | 0.48428E-04 |
| 86.94 | 4.8710 | 0.37097E-04 | 9.6162 | 0.24027E-04 | 19.0647 | 0.49966E-04 |
| 92.86 | 4.8721 | 0.38430E-04 | 9.6176 | 0.25398E-04 | 19.0703 | 0.51055E-04 |
| 98.78 | 4.8732 | 0.39820E-04 | 9.6191 | 0.26842E-04 | 19.0762 | 0.52171E-04 |
| 104.69 | 4.8744 | 0.41148E-04 | 9.6207 | 0.28301E-04 | 19.0821 | 0.53124E-04 |
| 110.61 | 4.8756 | 0.42363E-04 | 9.6224 | 0.29744E-04 | 19.0882 | 0.53840E-04 |
| 116.53 | 4.8768 | 0.43636E-04 | 9.6241 | 0.31290E-04 | 19.0943 | 0.54540E-04 |
| 122.45 | 4.8781 | 0.44755E-04 | 9.6259 | 0.32787E-04 | 19.1005 | 0.54958E-04 |
| 128.37 | 4.8794 | 0.45981E-04 | 9.6278 | 0.34423E-04 | 19.1068 | 0.55418E-04 |
| 134.29 | 4.8808 | 0.47138E-04 | 9.6298 | 0.36073E-04 | 19.1131 | 0.55696E-04 |
| 140.20 | 4.8822 | 0.48270E-04 | 9.6319 | 0.37770E-04 | 19.1194 | 0.55848E-04 |
| 146.12 | 4.8836 | 0.49442E-04 | 9.6341 | 0.39561E-04 | 19.1257 | 0.55953E-04 |
| 152.04 | 4.8850 | 0.50521E-04 | 9.6365 | 0.41345E-04 | 19.1321 | 0.55850E-04 |
| 157.96 | 4.8865 | 0.51623E-04 | 9.6389 | 0.43215E-04 | 19.1384 | 0.55672E-04 |
| 163.88 | 4.8880 | 0.52771E-04 | 9.6414 | 0.45193E-04 | 19.1447 | 0.55439E-04 |
| 169.80 | 4.8895 | 0.53988E-04 | 9.6440 | 0.47301E-04 | 19.1509 | 0.55168E-04 |
| 175.71 | 4.8911 | 0.55157E-04 | 9.6468 | 0.49439E-04 | 19.1572 | 0.54740E-04 |
| 181.63 | 4.8927 | 0.56396E-04 | 9.6497 | 0.51720E-04 | 19.1634 | 0.54260E-04 |
| 187.55 | 4.8944 | 0.57615E-04 | 9.6527 | 0.54059E-04 | 19.1695 | 0.53643E-04 |
| 193.47 | 4.8961 | 0.58862E-04 | 9.6558 | 0.56504E-04 | 19.1756 | 0.52929E-04 |
| 199.39 | 4.8978 | 0.60188E-04 | 9.6591 | 0.59106E-04 | 19.1815 | 0.52161E-04 |
| 205.31 | 4.8996 | 0.61494E-04 | 9.6626 | 0.61779E-04 | 19.1874 | 0.51235E-04 |
| 211.22 | 4.9014 | 0.62931E-04 | 9.6662 | 0.64669E-04 | 19.1931 | 0.50285E-04 |
| 217.14 | 4.9032 | 0.64404E-04 | 9.6700 | 0.67692E-04 | 19.1988 | 0.49214E-04 |
| 223.06 | 4.9051 | 0.65913E-04 | 9.6740 | 0.70851E-04 | 19.2043 | 0.48017E-04 |
| 228.98 | 4.9070 | 0.67461E-04 | 9.6781 | 0.74152E-04 | 19.2097 | 0.46691E-04 |
| 234.90 | 4.9090 | 0.69049E-04 | 9.6824 | 0.77601E-04 | 19.2150 | 0.45229E-04 |
| 240.82 | 4.9111 | 0.70779E-04 | 9.6870 | 0.81324E-04 | 19.2200 | 0.43680E-04 |
| 246.73 | 4.9131 | 0.72609E-04 | 9.6918 | 0.85278E-04 | 19.2249 | 0.42007E-04 |
| 252.65 | 4.9153 | 0.74489E-04 | 9.6968 | 0.89411E-04 | 19.2296 | 0.40173E-04 |
| 258.57 | 4.9175 | 0.76474E-04 | 9.7020 | 0.93799E-04 | 19.2340 | 0.38186E-04 |
| 264.49 | 4.9197 | 0.78461E-04 | 9.7075 | 0.98325E-04 | 19.2383 | 0.35984E-04 |
| 270.41 | 4.9220 | 0.80718E-04 | 9.7133 | 0.10334E-03 | 19.2422 | 0.33670E-04 |
| 276.33 | 4.9244 | 0.83098E-04 | 9.7194 | 0.10865E-03 | 19.2459 | 0.31163E-04 |
| 282.24 | 4.9269 | 0.85548E-04 | 9.7258 | 0.11423E-03 | 19.2494 | 0.28419E-04 |
| 288.16 | 4.9294 | 0.88239E-04 | 9.7325 | 0.12030E-03 | 19.2524 | 0.25467E-04 |
| 294.08 | 4.9320 | 0.91037E-04 | 9.7396 | 0.12667E-03 | 19.2552 | 0.22281E-04 |
| 300.00 | 4.9347 | 0.90955E-04 | 9.7471 | 0.12652E-03 | 19.2575 | 0.22287E-04 |

**POLMET**

Optimized Geometry:

SPACE GROUP (CENTROSYMMETRIC) : P -1

4.717798 9.635176 17.253347 106.953 98.917 98.865

O 0.434826 -0.375102 0.307134
O 0.265967 -0.021531 0.415913
N 0.185631 -0.166718 -0.465256
H 0.069921 -0.084646 -0.459036
C 0.326046 -0.243742 0.312832
H 0.099606 -0.270064 0.277653
H 0.460099 -0.169877 0.288742
C 0.346609 -0.160173 0.406638
H -0.425663 -0.144941 0.438018
C 0.151488 -0.252472 0.446672
H 0.226501 -0.355168 0.441847
C 0.105672 -0.254145 -0.411815
H 0.253493 -0.329901 -0.411723
C 0.150037 -0.145836 -0.322603
H 0.378720 -0.090523 -0.299255
H 0.083567 -0.205664 -0.282022
H 0.018403 -0.062916 -0.322922
C -0.464137 -0.439326 0.238284
C -0.341242 0.437054 0.238396
H -0.336195 0.399175 0.291463
C -0.227933 0.367340 0.172063
C -0.231506 0.417437 0.103896
C -0.469331 -0.388551 0.170462
H 0.434934 -0.295170 0.167633
C -0.350233 -0.459704 0.104758
H -0.351202 -0.417017 0.053543
C -0.268621 0.173865 -0.011748
H -0.261106 0.113652 0.033143
H 0.499436 0.168447 -0.036264
H 0.447924 0.055361 0.428828
H -0.075457 -0.281853 0.412305
C -0.212341 -0.347579 -0.442420
H -0.131997 0.273112 0.172918
C -0.105817 0.338333 0.031147
O -0.126594 0.111125 -0.076477
H -0.363371 -0.276040 -0.448487
H -0.268002 -0.402959 -0.398734
H -0.236653 -0.430512 0.497793
H -0.122225 0.394179 -0.014854
H 0.124785 0.341084 0.052178
C -0.265056 -0.037893 -0.123963
H -0.496040 -0.047468 -0.151046
H -0.255378 -0.112601 -0.086766

H -0.151259 -0.074266 -0.174471

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THERMAL PROPERTIES FROM HELMHOLTZ FREE ENERGY

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| T (K) | V (Ang^3) | Bt (GPa) | ALPHA (1/K) | Cp-Cv (J/mol*K) | Bs (GPa) | Sp-Sv (J/mol*K) |
|---|---|---|---|---|---|---|
| 10.00 | 748.6849 | 10.336 | 0.18198E-04 | 0.015 | 10.367 | 0.556 |
| 15.92 | 748.7342 | 10.315 | 0.18095E-04 | 0.024 | 10.329 | 2.122 |
| 21.84 | 748.8461 | 10.280 | 0.31502E-04 | 0.100 | 10.308 | 4.018 |
| 27.76 | 749.0119 | 10.235 | 0.43537E-04 | 0.243 | 10.278 | 5.854 |
| 33.67 | 749.2314 | 10.183 | 0.55310E-04 | 0.473 | 10.245 | 7.545 |
| 39.59 | 749.5002 | 10.124 | 0.65389E-04 | 0.774 | 10.205 | 9.091 |
| 45.51 | 749.8093 | 10.062 | 0.73774E-04 | 1.125 | 10.160 | 10.508 |
| 51.43 | 750.1542 | 9.997 | 0.81896E-04 | 1.558 | 10.112 | 11.816 |
| 57.35 | 750.5349 | 9.928 | 0.88830E-04 | 2.031 | 10.060 | 13.038 |
| 63.27 | 750.9426 | 9.857 | 0.95333E-04 | 2.563 | 10.007 | 14.186 |
| 69.18 | 751.3816 | 9.784 | 0.10132E-03 | 3.144 | 9.950 | 15.278 |
| 75.10 | 751.8430 | 9.709 | 0.10671E-03 | 3.760 | 9.891 | 16.319 |
| 81.02 | 752.3313 | 9.632 | 0.11234E-03 | 4.463 | 9.831 | 17.322 |
| 86.94 | 752.8419 | 9.554 | 0.11662E-03 | 5.122 | 9.766 | 18.292 |
| 92.86 | 753.3705 | 9.474 | 0.12100E-03 | 5.844 | 9.700 | 19.233 |
| 98.78 | 753.9215 | 9.393 | 0.12523E-03 | 6.606 | 9.633 | 20.153 |
| 104.69 | 754.4904 | 9.310 | 0.12936E-03 | 7.411 | 9.564 | 21.053 |
| 110.61 | 755.0772 | 9.226 | 0.13327E-03 | 8.242 | 9.494 | 21.938 |
| 116.53 | 755.6820 | 9.140 | 0.13698E-03 | 9.095 | 9.421 | 22.812 |
| 122.45 | 756.3046 | 9.053 | 0.14077E-03 | 10.005 | 9.347 | 23.677 |
| 128.37 | 756.9408 | 8.965 | 0.14426E-03 | 10.916 | 9.271 | 24.533 |
| 134.29 | 757.5992 | 8.874 | 0.14778E-03 | 11.873 | 9.193 | 25.390 |
| 140.20 | 758.2667 | 8.782 | 0.15124E-03 | 12.861 | 9.113 | 26.238 |
| 146.12 | 758.9555 | 8.688 | 0.15459E-03 | 13.867 | 9.031 | 27.091 |
| 152.04 | 759.6569 | 8.593 | 0.15809E-03 | 14.938 | 8.947 | 27.942 |
| 157.96 | 760.3768 | 8.495 | 0.16148E-03 | 16.022 | 8.861 | 28.797 |
| 163.88 | 761.1105 | 8.395 | 0.16491E-03 | 17.150 | 8.772 | 29.656 |
| 169.80 | 761.8627 | 8.293 | 0.16853E-03 | 18.349 | 8.681 | 30.521 |
| 175.71 | 762.6287 | 8.189 | 0.17224E-03 | 19.606 | 8.589 | 31.392 |
| 181.63 | 763.4178 | 8.082 | 0.17575E-03 | 20.845 | 8.491 | 32.277 |
| 187.55 | 764.2208 | 7.972 | 0.17944E-03 | 22.157 | 8.392 | 33.168 |
| 193.47 | 765.0375 | 7.859 | 0.18331E-03 | 23.541 | 8.290 | 34.067 |
| 199.39 | 765.8774 | 7.743 | 0.18739E-03 | 25.005 | 8.184 | 34.983 |
| 205.31 | 766.7403 | 7.623 | 0.19186E-03 | 26.602 | 8.075 | 35.917 |
| 211.22 | 767.6171 | 7.500 | 0.19621E-03 | 28.193 | 7.962 | 36.860 |
| 217.14 | 768.5216 | 7.372 | 0.20084E-03 | 29.884 | 7.844 | 37.827 |
| 223.06 | 769.4445 | 7.240 | 0.20587E-03 | 31.714 | 7.722 | 38.810 |
| 228.98 | 770.3951 | 7.102 | 0.21117E-03 | 33.644 | 7.594 | 39.817 |
| 234.90 | 771.3688 | 6.959 | 0.21696E-03 | 35.744 | 7.462 | 40.846 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 240.82 | 772.3747 | 6.809 | 0.22323E-03 | 38.006 | 7.322 | 41.905 |
| 246.73 | 773.4084 | 6.652 | 0.22999E-03 | 40.435 | 7.176 | 42.991 |
| 252.65 | 774.4790 | 6.487 | 0.23721E-03 | 43.011 | 7.020 | 44.113 |
| 258.57 | 775.5819 | 6.313 | 0.24550E-03 | 45.951 | 6.858 | 45.268 |
| 264.49 | 776.7263 | 6.129 | 0.25475E-03 | 49.207 | 6.685 | 46.466 |
| 270.41 | 777.9215 | 5.931 | 0.26517E-03 | 52.836 | 6.500 | 47.715 |
| 276.33 | 779.1674 | 5.720 | 0.27723E-03 | 57.004 | 6.301 | 49.018 |
| 282.24 | 780.4687 | 5.493 | 0.29102E-03 | 61.712 | 6.087 | 50.380 |
| 288.16 | 781.8485 | 5.244 | 0.30780E-03 | 67.410 | 5.853 | 51.826 |
| 294.08 | 783.3067 | 4.971 | 0.32684E-03 | 73.665 | 5.591 | 53.357 |
| 300.00 | 784.8757 | 4.665 | 0.32585E-03 | 70.234 | 5.211 | 55.008 |

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LINEAR THERMAL EXPANSION OF CONVENTIONAL LATTICE PARAMETERS

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| T (K) | a (Ang) | ALPHA_a (1/K) | b (Ang) | ALPHA_b (1/K) | c (Ang) | ALPHA_c (1/K) |
|---|---|---|---|---|---|---|
| 10.00 | 4.7727 | 0.59325E-05 | 9.7570 | 0.68243E-05 | 17.4059 | 0.56989E-05 |
| 15.92 | 4.7728 | 0.58987E-05 | 9.7573 | 0.67857E-05 | 17.4063 | 0.56687E-05 |
| 21.84 | 4.7731 | 0.10263E-04 | 9.7578 | 0.11809E-04 | 17.4071 | 0.98860E-05 |
| 27.76 | 4.7734 | 0.14162E-04 | 9.7586 | 0.16305E-04 | 17.4083 | 0.13722E-04 |
| 33.67 | 4.7739 | 0.17954E-04 | 9.7597 | 0.20688E-04 | 17.4099 | 0.17531E-04 |
| 39.59 | 4.7744 | 0.21171E-04 | 9.7610 | 0.24419E-04 | 17.4119 | 0.20871E-04 |
| 45.51 | 4.7751 | 0.23815E-04 | 9.7625 | 0.27498E-04 | 17.4142 | 0.23739E-04 |
| 51.43 | 4.7758 | 0.26346E-04 | 9.7642 | 0.30459E-04 | 17.4168 | 0.26597E-04 |
| 57.35 | 4.7765 | 0.28469E-04 | 9.7660 | 0.32958E-04 | 17.4197 | 0.29144E-04 |
| 63.27 | 4.7774 | 0.30425E-04 | 9.7680 | 0.35273E-04 | 17.4228 | 0.31631E-04 |
| 69.18 | 4.7783 | 0.32191E-04 | 9.7701 | 0.37375E-04 | 17.4262 | 0.34025E-04 |
| 75.10 | 4.7792 | 0.33737E-04 | 9.7723 | 0.39232E-04 | 17.4298 | 0.36305E-04 |
| 81.02 | 4.7802 | 0.35330E-04 | 9.7746 | 0.41153E-04 | 17.4337 | 0.38753E-04 |
| 86.94 | 4.7812 | 0.36470E-04 | 9.7771 | 0.42552E-04 | 17.4378 | 0.40823E-04 |
| 92.86 | 4.7822 | 0.37599E-04 | 9.7796 | 0.43948E-04 | 17.4421 | 0.43053E-04 |
| 98.78 | 4.7833 | 0.38667E-04 | 9.7822 | 0.45276E-04 | 17.4467 | 0.45286E-04 |
| 104.69 | 4.7844 | 0.39672E-04 | 9.7848 | 0.46536E-04 | 17.4515 | 0.47575E-04 |
| 110.61 | 4.7856 | 0.40580E-04 | 9.7876 | 0.47688E-04 | 17.4565 | 0.49888E-04 |
| 116.53 | 4.7867 | 0.41395E-04 | 9.7903 | 0.48735E-04 | 17.4618 | 0.52225E-04 |
| 122.45 | 4.7879 | 0.42201E-04 | 9.7932 | 0.49777E-04 | 17.4673 | 0.54706E-04 |
| 128.37 | 4.7891 | 0.42885E-04 | 9.7961 | 0.50678E-04 | 17.4731 | 0.57179E-04 |
| 134.29 | 4.7903 | 0.43544E-04 | 9.7991 | 0.51554E-04 | 17.4792 | 0.59787E-04 |
| 140.20 | 4.7916 | 0.44149E-04 | 9.8021 | 0.52369E-04 | 17.4855 | 0.62491E-04 |
| 146.12 | 4.7929 | 0.44681E-04 | 9.8052 | 0.53101E-04 | 17.4921 | 0.65281E-04 |
| 152.04 | 4.7941 | 0.45222E-04 | 9.8083 | 0.53846E-04 | 17.4990 | 0.68268E-04 |
| 157.96 | 4.7954 | 0.45684E-04 | 9.8114 | 0.54500E-04 | 17.5062 | 0.71354E-04 |
| 163.88 | 4.7967 | 0.46120E-04 | 9.8146 | 0.55124E-04 | 17.5138 | 0.74612E-04 |
| 169.80 | 4.7980 | 0.46557E-04 | 9.8178 | 0.55752E-04 | 17.5217 | 0.78124E-04 |
| 175.71 | 4.7994 | 0.46974E-04 | 9.8211 | 0.56357E-04 | 17.5300 | 0.81857E-04 |

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|---|---|---|---|---|---|---|
| 181.63 | 4.8007 | 0.47282E-04 | 9.8244 | 0.56833E-04 | 17.5387 | 0.85674E-04 |
| 187.55 | 4.8021 | 0.47585E-04 | 9.8277 | 0.57304E-04 | 17.5478 | 0.89783E-04 |
| 193.47 | 4.8034 | 0.47871E-04 | 9.8310 | 0.57754E-04 | 17.5573 | 0.94208E-04 |
| 199.39 | 4.8048 | 0.48150E-04 | 9.8344 | 0.58196E-04 | 17.5673 | 0.98964E-04 |
| 205.31 | 4.8062 | 0.48458E-04 | 9.8378 | 0.58673E-04 | 17.5779 | 0.10419E-03 |
| 211.22 | 4.8075 | 0.48657E-04 | 9.8412 | 0.59018E-04 | 17.5890 | 0.10964E-03 |
| 217.14 | 4.8089 | 0.48840E-04 | 9.8447 | 0.59343E-04 | 17.6007 | 0.11555E-03 |
| 223.06 | 4.8103 | 0.49031E-04 | 9.8482 | 0.59675E-04 | 17.6130 | 0.12203E-03 |
| 228.98 | 4.8117 | 0.49179E-04 | 9.8516 | 0.59954E-04 | 17.6261 | 0.12905E-03 |
| 234.90 | 4.8131 | 0.49329E-04 | 9.8551 | 0.60232E-04 | 17.6399 | 0.13680E-03 |
| 240.82 | 4.8145 | 0.49454E-04 | 9.8587 | 0.60477E-04 | 17.6546 | 0.14533E-03 |
| 246.73 | 4.8159 | 0.49542E-04 | 9.8622 | 0.60672E-04 | 17.6702 | 0.15472E-03 |
| 252.65 | 4.8173 | 0.49562E-04 | 9.8658 | 0.60779E-04 | 17.6869 | 0.16503E-03 |
| 258.57 | 4.8188 | 0.49610E-04 | 9.8693 | 0.60913E-04 | 17.7047 | 0.17682E-03 |
| 264.49 | 4.8202 | 0.49622E-04 | 9.8729 | 0.60994E-04 | 17.7238 | 0.19014E-03 |
| 270.41 | 4.8216 | 0.49597E-04 | 9.8764 | 0.61019E-04 | 17.7445 | 0.20531E-03 |
| 276.33 | 4.8230 | 0.49545E-04 | 9.8800 | 0.60996E-04 | 17.7669 | 0.22298E-03 |
| 282.24 | 4.8244 | 0.49400E-04 | 9.8836 | 0.60838E-04 | 17.7911 | 0.24352E-03 |
| 288.16 | 4.8258 | 0.49253E-04 | 9.8871 | 0.60650E-04 | 17.8179 | 0.26846E-03 |
| 294.08 | 4.8272 | 0.49061E-04 | 9.8907 | 0.60387E-04 | 17.8474 | 0.29685E-03 |
| 300.00 | 4.8286 | 0.49029E-04 | 9.8942 | 0.60346E-04 | 17.8805 | 0.29587E-03 |

**KAZPOQ**

Optimized Geometry:

SPACE GROUP (CENTROSYMMETRIC) : P -1

5.315333 7.482334 16.137790 94.933 97.369 94.009

| | | | |
|---|---|---|---|
| O | -0.295390 | 0.160293 | 0.239127 |
| O | -0.262160 | -0.023941 | 0.073996 |
| H | -0.431901 | -0.090485 | 0.071075 |
| N | 0.493329 | 0.414153 | -0.360629 |
| N | -0.242281 | 0.178440 | -0.060674 |
| H | -0.139700 | 0.069661 | -0.067495 |
| C | 0.293917 | 0.350034 | -0.382423 |
| C | 0.032156 | 0.265630 | -0.409735 |
| H | -0.101131 | 0.348589 | -0.381105 |
| H | 0.017715 | 0.134228 | -0.385240 |
| C | -0.041634 | 0.243775 | 0.495156 |
| C | -0.281603 | 0.160062 | 0.464029 |
| H | -0.404962 | 0.118275 | -0.492022 |
| C | -0.361996 | 0.132522 | 0.379160 |
| H | 0.452435 | 0.067457 | 0.355098 |
| C | -0.202670 | 0.192233 | 0.322316 |
| C | 0.035095 | 0.278553 | 0.353224 |

| | | | |
|---|---|---|---|
| H | 0.161929 | 0.328885 | 0.312050 |
| C | 0.113750 | 0.303225 | 0.439443 |
| H | 0.299212 | 0.371040 | 0.461691 |
| C | -0.153075 | 0.234393 | 0.179756 |
| H | 0.041644 | 0.193637 | 0.186887 |
| H | -0.143114 | 0.381684 | 0.187679 |
| C | -0.287179 | 0.162244 | 0.089946 |
| H | -0.487427 | 0.189841 | 0.086128 |
| C | -0.163370 | 0.268653 | 0.024138 |
| H | -0.224669 | 0.404099 | 0.027420 |
| H | 0.043146 | 0.280047 | 0.040051 |
| C | -0.205164 | 0.294490 | -0.128374 |
| H | -0.024156 | 0.375633 | -0.113933 |
| C | -0.422110 | 0.422187 | -0.138846 |
| H | 0.396833 | 0.343766 | -0.156667 |
| H | -0.392836 | -0.490441 | -0.187561 |
| H | -0.429645 | -0.495293 | -0.080969 |
| C | -0.202189 | 0.173528 | -0.210863 |
| H | -0.030757 | 0.102600 | -0.207261 |
| H | -0.208734 | 0.254911 | -0.263189 |
| H | -0.367293 | 0.076519 | -0.221118 |

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THERMAL PROPERTIES FROM HELMHOLTZ FREE ENERGY

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| T (K) | V (Ang^3) | Bt (GPa) | ALPHA (1/K) | Cp-Cv (J/mol*K) | Bs (GPa) | Sp-Sv (J/mol*K) |
|---|---|---|---|---|---|---|
| 10.00 | 648.5065 | 13.495 | 0.87364E-05 | 0.004 | 13.510 | 0.282 |
| 15.92 | 648.5271 | 13.489 | 0.87361E-05 | 0.006 | 13.495 | 1.017 |
| 21.84 | 648.5735 | 13.478 | 0.15343E-04 | 0.027 | 13.491 | 1.947 |
| 27.76 | 648.6457 | 13.462 | 0.22788E-04 | 0.076 | 13.485 | 2.955 |
| 33.67 | 648.7489 | 13.442 | 0.30678E-04 | 0.166 | 13.478 | 3.970 |
| 39.59 | 648.8805 | 13.420 | 0.37724E-04 | 0.295 | 13.470 | 4.950 |
| 45.51 | 649.0378 | 13.395 | 0.44038E-04 | 0.462 | 13.459 | 5.875 |
| 51.43 | 649.2183 | 13.369 | 0.50179E-04 | 0.677 | 13.449 | 6.738 |
| 57.35 | 649.4221 | 13.343 | 0.55141E-04 | 0.910 | 13.437 | 7.542 |
| 63.27 | 649.6414 | 13.316 | 0.59371E-04 | 1.162 | 13.424 | 8.290 |
| 69.18 | 649.8787 | 13.290 | 0.63820E-04 | 1.466 | 13.413 | 8.991 |
| 75.10 | 650.1314 | 13.264 | 0.67426E-04 | 1.773 | 13.400 | 9.650 |
| 81.02 | 650.3971 | 13.238 | 0.70749E-04 | 2.103 | 13.388 | 10.273 |
| 86.94 | 650.6757 | 13.213 | 0.73788E-04 | 2.451 | 13.375 | 10.865 |
| 92.86 | 650.9645 | 13.188 | 0.75881E-04 | 2.764 | 13.360 | 11.430 |
| 98.78 | 651.2612 | 13.164 | 0.78203E-04 | 3.119 | 13.347 | 11.972 |
| 104.69 | 651.5666 | 13.141 | 0.80330E-04 | 3.483 | 13.335 | 12.494 |
| 110.61 | 651.8823 | 13.117 | 0.82372E-04 | 3.865 | 13.323 | 13.001 |
| 116.53 | 652.2033 | 13.095 | 0.84165E-04 | 4.246 | 13.311 | 13.492 |
| 122.45 | 652.5322 | 13.073 | 0.85693E-04 | 4.619 | 13.298 | 13.972 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 128.37 | 652.8663 | 13.052 | 0.87152E-04 | 5.003 | 13.286 | 14.440 |
| 134.29 | 653.2057 | 13.031 | 0.88468E-04 | 5.387 | 13.274 | 14.898 |
| 140.20 | 653.5503 | 13.010 | 0.89783E-04 | 5.787 | 13.262 | 15.349 |
| 146.12 | 653.9003 | 12.990 | 0.90963E-04 | 6.185 | 13.251 | 15.792 |
| 152.04 | 654.2554 | 12.971 | 0.91940E-04 | 6.568 | 13.238 | 16.230 |
| 157.96 | 654.6133 | 12.952 | 0.92841E-04 | 6.952 | 13.226 | 16.661 |
| 163.88 | 654.9737 | 12.933 | 0.93670E-04 | 7.335 | 13.214 | 17.087 |
| 169.80 | 655.3394 | 12.915 | 0.94502E-04 | 7.729 | 13.203 | 17.509 |
| 175.71 | 655.7077 | 12.897 | 0.95267E-04 | 8.121 | 13.191 | 17.928 |
| 181.63 | 656.0787 | 12.879 | 0.96022E-04 | 8.522 | 13.180 | 18.342 |
| 187.55 | 656.4523 | 12.862 | 0.96715E-04 | 8.920 | 13.169 | 18.754 |
| 193.47 | 656.8311 | 12.845 | 0.97340E-04 | 9.314 | 13.158 | 19.165 |
| 199.39 | 657.2100 | 12.828 | 0.97894E-04 | 9.701 | 13.147 | 19.571 |
| 205.31 | 657.5915 | 12.812 | 0.98375E-04 | 10.081 | 13.135 | 19.976 |
| 211.22 | 657.9756 | 12.796 | 0.98993E-04 | 10.495 | 13.125 | 20.379 |
| 217.14 | 658.3624 | 12.780 | 0.99479E-04 | 10.888 | 13.113 | 20.781 |
| 223.06 | 658.7517 | 12.764 | 0.99894E-04 | 11.271 | 13.102 | 21.182 |
| 228.98 | 659.1411 | 12.749 | 0.10030E-03 | 11.659 | 13.091 | 21.581 |
| 234.90 | 659.5331 | 12.734 | 0.10065E-03 | 12.035 | 13.080 | 21.978 |
| 240.82 | 659.9278 | 12.719 | 0.10106E-03 | 12.433 | 13.069 | 22.376 |
| 246.73 | 660.3224 | 12.705 | 0.10147E-03 | 12.835 | 13.058 | 22.771 |
| 252.65 | 660.7197 | 12.690 | 0.10181E-03 | 13.224 | 13.047 | 23.166 |
| 258.57 | 661.1196 | 12.676 | 0.10209E-03 | 13.602 | 13.036 | 23.562 |
| 264.49 | 661.5195 | 12.662 | 0.10230E-03 | 13.962 | 13.024 | 23.955 |
| 270.41 | 661.9194 | 12.648 | 0.10257E-03 | 14.343 | 13.013 | 24.347 |
| 276.33 | 662.3219 | 12.634 | 0.10291E-03 | 14.747 | 13.003 | 24.740 |
| 282.24 | 662.7271 | 12.621 | 0.10319E-03 | 15.137 | 12.992 | 25.132 |
| 288.16 | 663.1323 | 12.607 | 0.10339E-03 | 15.509 | 12.981 | 25.524 |
| 294.08 | 663.5375 | 12.594 | 0.10354E-03 | 15.867 | 12.969 | 25.914 |
| 300.00 | 663.9452 | 12.581 | 0.10344E-03 | 16.149 | 12.956 | 26.305 |

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LINEAR THERMAL EXPANSION OF CONVENTIONAL LATTICE PARAMETERS

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| T (K) | a (Ang) | ALPHA_a (1/K) | b (Ang) | ALPHA_b (1/K) | c (Ang) | ALPHA_c (1/K) |
|---|---|---|---|---|---|---|
| 10.00 | 5.3453 | 0.12276E-05 | 7.5992 | 0.62066E-05 | 16.2182 | 0.16529E-05 |
| 15.92 | 5.3453 | 0.12267E-05 | 7.5994 | 0.62077E-05 | 16.2183 | 0.16527E-05 |
| 21.84 | 5.3454 | 0.21474E-05 | 7.5998 | 0.10914E-04 | 16.2185 | 0.29009E-05 |
| 27.76 | 5.3454 | 0.31597E-05 | 7.6004 | 0.16257E-04 | 16.2189 | 0.43010E-05 |
| 33.67 | 5.3456 | 0.41984E-05 | 7.6013 | 0.21975E-04 | 16.2194 | 0.57761E-05 |
| 39.59 | 5.3457 | 0.50745E-05 | 7.6024 | 0.27163E-04 | 16.2200 | 0.70802E-05 |
| 45.51 | 5.3459 | 0.57997E-05 | 7.6037 | 0.31909E-04 | 16.2207 | 0.82331E-05 |
| 51.43 | 5.3461 | 0.64415E-05 | 7.6052 | 0.36628E-04 | 16.2215 | 0.93376E-05 |
| 57.35 | 5.3463 | 0.68735E-05 | 7.6070 | 0.40580E-04 | 16.2225 | 0.10207E-04 |
| 63.27 | 5.3465 | 0.71529E-05 | 7.6089 | 0.44093E-04 | 16.2235 | 0.10923E-04 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 69.18 | 5.3467 | 0.73996E-05 | 7.6110 | 0.47866E-04 | 16.2246 | 0.11663E-04 |
| 75.10 | 5.3470 | 0.74854E-05 | 7.6132 | 0.51110E-04 | 16.2257 | 0.12230E-04 |
| 81.02 | 5.3472 | 0.74786E-05 | 7.6156 | 0.54240E-04 | 16.2269 | 0.12727E-04 |
| 86.94 | 5.3474 | 0.73828E-05 | 7.6181 | 0.57250E-04 | 16.2282 | 0.13155E-04 |
| 92.86 | 5.3477 | 0.71180E-05 | 7.6207 | 0.59648E-04 | 16.2295 | 0.13390E-04 |
| 98.78 | 5.3479 | 0.68434E-05 | 7.6235 | 0.62280E-04 | 16.2308 | 0.13656E-04 |
| 104.69 | 5.3481 | 0.64988E-05 | 7.6263 | 0.64843E-04 | 16.2321 | 0.13870E-04 |
| 110.61 | 5.3483 | 0.60943E-05 | 7.6293 | 0.67427E-04 | 16.2334 | 0.14051E-04 |
| 116.53 | 5.3485 | 0.56182E-05 | 7.6324 | 0.69896E-04 | 16.2348 | 0.14172E-04 |
| 122.45 | 5.3487 | 0.50726E-05 | 7.6357 | 0.72232E-04 | 16.2362 | 0.14229E-04 |
| 128.37 | 5.3488 | 0.44748E-05 | 7.6390 | 0.74591E-04 | 16.2375 | 0.14258E-04 |
| 134.29 | 5.3490 | 0.38194E-05 | 7.6424 | 0.76912E-04 | 16.2389 | 0.14246E-04 |
| 140.20 | 5.3491 | 0.31151E-05 | 7.6459 | 0.79314E-04 | 16.2403 | 0.14215E-04 |
| 146.12 | 5.3491 | 0.23589E-05 | 7.6496 | 0.81677E-04 | 16.2416 | 0.14145E-04 |
| 152.04 | 5.3492 | 0.15521E-05 | 7.6533 | 0.83933E-04 | 16.2430 | 0.14026E-04 |
| 157.96 | 5.3492 | 0.69722E-06 | 7.6572 | 0.86200E-04 | 16.2443 | 0.13878E-04 |
| 163.88 | 5.3493 | -0.20276E-06 | 7.6611 | 0.88475E-04 | 16.2457 | 0.13701E-04 |
| 169.80 | 5.3492 | -0.11446E-05 | 7.6652 | 0.90824E-04 | 16.2470 | 0.13508E-04 |
| 175.71 | 5.3492 | -0.21286E-05 | 7.6694 | 0.93180E-04 | 16.2483 | 0.13289E-04 |
| 181.63 | 5.3491 | -0.31609E-05 | 7.6737 | 0.95609E-04 | 16.2495 | 0.13048E-04 |
| 187.55 | 5.3490 | -0.42324E-05 | 7.6781 | 0.98044E-04 | 16.2508 | 0.12783E-04 |
| 193.47 | 5.3488 | -0.53430E-05 | 7.6826 | 0.10048E-03 | 16.2520 | 0.12491E-04 |
| 199.39 | 5.3486 | -0.64929E-05 | 7.6872 | 0.10292E-03 | 16.2532 | 0.12172E-04 |
| 205.31 | 5.3484 | -0.76822E-05 | 7.6919 | 0.10535E-03 | 16.2543 | 0.11826E-04 |
| 211.22 | 5.3482 | -0.89227E-05 | 7.6968 | 0.10800E-03 | 16.2554 | 0.11480E-04 |
| 217.14 | 5.3479 | -0.10193E-04 | 7.7018 | 0.11057E-03 | 16.2565 | 0.11101E-04 |
| 223.06 | 5.3475 | -0.11497E-04 | 7.7069 | 0.11314E-03 | 16.2576 | 0.10696E-04 |
| 228.98 | 5.3471 | -0.12845E-04 | 7.7121 | 0.11577E-03 | 16.2586 | 0.10272E-04 |
| 234.90 | 5.3467 | -0.14222E-04 | 7.7174 | 0.11838E-03 | 16.2596 | 0.98253E-05 |
| 240.82 | 5.3462 | -0.15648E-04 | 7.7229 | 0.12114E-03 | 16.2605 | 0.93683E-05 |
| 246.73 | 5.3457 | -0.17119E-04 | 7.7285 | 0.12397E-03 | 16.2614 | 0.88915E-05 |
| 252.65 | 5.3451 | -0.18619E-04 | 7.7343 | 0.12679E-03 | 16.2622 | 0.83914E-05 |
| 258.57 | 5.3445 | -0.20144E-04 | 7.7401 | 0.12958E-03 | 16.2630 | 0.78705E-05 |
| 264.49 | 5.3439 | -0.21696E-04 | 7.7461 | 0.13235E-03 | 16.2637 | 0.73258E-05 |
| 270.41 | 5.3432 | -0.23304E-04 | 7.7523 | 0.13527E-03 | 16.2644 | 0.67671E-05 |
| 276.33 | 5.3424 | -0.24965E-04 | 7.7585 | 0.13834E-03 | 16.2650 | 0.61967E-05 |
| 282.24 | 5.3416 | -0.26648E-04 | 7.7650 | 0.14138E-03 | 16.2656 | 0.56060E-05 |
| 288.16 | 5.3407 | -0.28358E-04 | 7.7715 | 0.14439E-03 | 16.2661 | 0.49921E-05 |
| 294.08 | 5.3398 | -0.30107E-04 | 7.7782 | 0.14742E-03 | 16.2665 | 0.43535E-05 |
| 300.00 | 5.3388 | -0.30101E-04 | 7.7851 | 0.14724E-03 | 16.2669 | 0.43528E-05 |

**PROPRA10**

Optimized Geometry:

SPACE GROUP (CENTROSYMMETRIC) : P 21/C

11.367849 4.348493 26.389340 90.000 100.041 90.000

C 0.176571 0.169309 -0.177134
C 0.120005 0.039040 -0.221653
C 0.157453 0.113506 -0.268985
C 0.246567 0.317269 -0.270877
C 0.307623 0.456047 -0.224588
C 0.401857 -0.327314 -0.224472
C 0.459080 -0.203839 -0.179718
C 0.426716 -0.290022 -0.132006
C 0.336691 -0.493222 -0.131175
C 0.274395 0.378585 -0.177713
C 0.051955 -0.076134 -0.124344
C 0.048563 -0.084812 -0.065279
C 0.167271 -0.231148 -0.037388
C 0.284277 -0.352695 0.048704
C 0.285638 -0.277119 0.106242
C 0.396571 -0.220415 0.030545
O 0.147459 0.123606 -0.129914
O -0.051751 -0.251146 -0.055180
N 0.172317 -0.229743 0.018554
H 0.047246 -0.119438 -0.221976
H 0.112079 0.003986 -0.303667
H 0.273520 0.376380 -0.306788
H 0.426028 -0.260247 -0.260622
H -0.470549 -0.038009 -0.179755
H 0.474071 -0.190940 -0.096879
H 0.310338 0.436844 -0.095632
H -0.033061 0.009028 -0.145772
H 0.067186 -0.307901 -0.138073
H 0.046163 0.153758 -0.052436
H -0.108760 -0.106038 -0.043434
H 0.174572 -0.462086 -0.052585
H 0.239963 -0.095140 -0.047361
H 0.104111 -0.361001 0.027133
H 0.286924 0.398121 0.044698
H 0.206109 -0.369146 0.118189
H 0.363593 -0.376936 0.130075
H 0.287463 -0.030219 0.111742
H 0.475461 -0.283022 0.057867
H 0.405746 -0.310728 -0.006784
H 0.391614 0.027659 0.027973

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THERMAL PROPERTIES FROM HELMHOLTZ FREE ENERGY

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T (K) V (Ang^3) Bt (GPa) ALPHA (1/K) Cp-Cv (J/mol*K) Bs (GPa) Sp-Sv (J/mol*K)

| | | | | | | |
|---|---|---|---|---|---|---|
| 10.00 | 1320.2653 | 12.474 | 0.19314E-04 | 0.037 | 12.505 | 2.022 |
| 15.92 | 1320.3686 | 12.454 | 0.19312E-04 | 0.059 | 12.473 | 4.612 |
| 21.84 | 1320.5672 | 12.420 | 0.31590E-04 | 0.215 | 12.458 | 7.631 |
| 27.76 | 1320.8611 | 12.376 | 0.43437E-04 | 0.516 | 12.437 | 10.650 |
| 33.67 | 1321.2423 | 12.324 | 0.53582E-04 | 0.948 | 12.408 | 13.441 |
| 39.59 | 1321.6951 | 12.268 | 0.62110E-04 | 1.491 | 12.374 | 15.951 |
| 45.51 | 1322.2114 | 12.207 | 0.69614E-04 | 2.144 | 12.336 | 18.204 |
| 51.43 | 1322.7833 | 12.144 | 0.76771E-04 | 2.932 | 12.297 | 20.246 |
| 57.35 | 1323.4107 | 12.078 | 0.82903E-04 | 3.794 | 12.253 | 22.124 |
| 63.27 | 1324.0780 | 12.011 | 0.87170E-04 | 4.604 | 12.202 | 23.871 |
| 69.18 | 1324.7769 | 11.943 | 0.91598E-04 | 5.531 | 12.152 | 25.513 |
| 75.10 | 1325.5156 | 11.873 | 0.96947E-04 | 6.690 | 12.106 | 27.080 |
| 81.02 | 1326.2940 | 11.802 | 0.10018E-03 | 7.665 | 12.049 | 28.592 |
| 86.94 | 1327.0883 | 11.731 | 0.10366E-03 | 8.758 | 11.994 | 30.045 |
| 92.86 | 1327.9223 | 11.658 | 0.10688E-03 | 9.890 | 11.936 | 31.470 |
| 98.78 | 1328.7722 | 11.585 | 0.11006E-03 | 11.091 | 11.879 | 32.857 |
| 104.69 | 1329.6539 | 11.510 | 0.11301E-03 | 12.323 | 11.819 | 34.226 |
| 110.61 | 1330.5515 | 11.435 | 0.11577E-03 | 13.584 | 11.758 | 35.570 |
| 116.53 | 1331.4808 | 11.359 | 0.11841E-03 | 14.882 | 11.696 | 36.908 |
| 122.45 | 1332.4180 | 11.283 | 0.12105E-03 | 16.244 | 11.633 | 38.224 |
| 128.37 | 1333.3871 | 11.205 | 0.12338E-03 | 17.582 | 11.567 | 39.541 |
| 134.29 | 1334.3720 | 11.127 | 0.12591E-03 | 19.035 | 11.502 | 40.850 |
| 140.20 | 1335.3728 | 11.048 | 0.12813E-03 | 20.449 | 11.435 | 42.153 |
| 146.12 | 1336.3975 | 10.968 | 0.13034E-03 | 21.912 | 11.366 | 43.459 |
| 152.04 | 1337.4380 | 10.887 | 0.13246E-03 | 23.390 | 11.295 | 44.764 |
| 157.96 | 1338.4944 | 10.805 | 0.13455E-03 | 24.907 | 11.224 | 46.069 |
| 163.88 | 1339.5667 | 10.723 | 0.13675E-03 | 26.507 | 11.152 | 47.375 |
| 169.80 | 1340.6628 | 10.639 | 0.13894E-03 | 28.155 | 11.079 | 48.693 |
| 175.71 | 1341.7748 | 10.554 | 0.14121E-03 | 29.881 | 11.005 | 50.015 |
| 181.63 | 1342.9027 | 10.468 | 0.14324E-03 | 31.551 | 10.928 | 51.343 |
| 187.55 | 1344.0537 | 10.381 | 0.14522E-03 | 33.237 | 10.850 | 52.684 |
| 193.47 | 1345.2158 | 10.293 | 0.14733E-03 | 35.017 | 10.771 | 54.029 |
| 199.39 | 1346.3942 | 10.204 | 0.14942E-03 | 36.832 | 10.690 | 55.384 |
| 205.31 | 1347.5972 | 10.114 | 0.15165E-03 | 38.753 | 10.608 | 56.756 |
| 211.22 | 1348.8165 | 10.022 | 0.15377E-03 | 40.659 | 10.524 | 58.139 |
| 217.14 | 1350.0522 | 9.929 | 0.15588E-03 | 42.591 | 10.438 | 59.534 |
| 223.06 | 1351.3043 | 9.834 | 0.15809E-03 | 44.612 | 10.351 | 60.941 |
| 228.98 | 1352.5809 | 9.737 | 0.16049E-03 | 46.781 | 10.262 | 62.368 |
| 234.90 | 1353.8739 | 9.639 | 0.16290E-03 | 48.987 | 10.172 | 63.809 |
| 240.82 | 1355.1914 | 9.539 | 0.16529E-03 | 51.219 | 10.079 | 65.272 |
| 246.73 | 1356.5253 | 9.438 | 0.16768E-03 | 53.482 | 9.983 | 66.749 |
| 252.65 | 1357.8838 | 9.334 | 0.17005E-03 | 55.763 | 9.885 | 68.249 |
| 258.57 | 1359.2586 | 9.228 | 0.17262E-03 | 58.202 | 9.785 | 69.764 |
| 264.49 | 1360.6579 | 9.120 | 0.17548E-03 | 60.866 | 9.684 | 71.303 |
| 270.41 | 1362.0819 | 9.009 | 0.17845E-03 | 63.635 | 9.581 | 72.866 |
| 276.33 | 1363.5385 | 8.895 | 0.18131E-03 | 66.349 | 9.473 | 74.461 |
| 282.24 | 1365.0115 | 8.779 | 0.18425E-03 | 69.149 | 9.362 | 76.074 |

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|---|---|---|---|---|---|---|
| 288.16 | 1366.5091 | 8.660 | 0.18738E-03 | 72.103 | 9.248 | 77.712 |
| 294.08 | 1368.0394 | 8.537 | 0.19103E-03 | 75.482 | 9.133 | 79.384 |
| 300.00 | 1369.6024 | 8.411 | 0.19081E-03 | 75.774 | 8.990 | 81.090 |

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LINEAR THERMAL EXPANSION OF CONVENTIONAL LATTICE PARAMETERS

**********

| T (K) | a (Ang) | ALPHA_a (1/K) | b (Ang) | ALPHA_b (1/K) | c (Ang) | ALPHA_c (1/K) |
|---|---|---|---|---|---|---|
| 10.00 | 11.4123 | 0.30662E-05 | 4.4098 | 0.92888E-05 | 26.5950 | 0.57280E-05 |
| 15.92 | 11.4125 | 0.30657E-05 | 4.4099 | 0.92892E-05 | 26.5956 | 0.57275E-05 |
| 21.84 | 11.4128 | 0.50108E-05 | 4.4103 | 0.15205E-04 | 26.5968 | 0.93657E-05 |
| 27.76 | 11.4132 | 0.68769E-05 | 4.4107 | 0.20941E-04 | 26.5986 | 0.12868E-04 |
| 33.67 | 11.4137 | 0.84613E-05 | 4.4113 | 0.25887E-04 | 26.6008 | 0.15857E-04 |
| 39.59 | 11.4143 | 0.97759E-05 | 4.4121 | 0.30087E-04 | 26.6035 | 0.18355E-04 |
| 45.51 | 11.4150 | 0.10913E-04 | 4.4129 | 0.33829E-04 | 26.6066 | 0.20539E-04 |
| 51.43 | 11.4158 | 0.11978E-04 | 4.4138 | 0.37448E-04 | 26.6100 | 0.22605E-04 |
| 57.35 | 11.4166 | 0.12862E-04 | 4.4149 | 0.40615E-04 | 26.6137 | 0.24354E-04 |
| 63.27 | 11.4175 | 0.13437E-04 | 4.4160 | 0.42915E-04 | 26.6176 | 0.25539E-04 |
| 69.18 | 11.4184 | 0.14016E-04 | 4.4171 | 0.45342E-04 | 26.6218 | 0.26755E-04 |
| 75.10 | 11.4194 | 0.14710E-04 | 4.4183 | 0.48285E-04 | 26.6261 | 0.28220E-04 |
| 81.02 | 11.4204 | 0.15059E-04 | 4.4196 | 0.50229E-04 | 26.6306 | 0.29049E-04 |
| 86.94 | 11.4214 | 0.15416E-04 | 4.4210 | 0.52362E-04 | 26.6352 | 0.29926E-04 |
| 92.86 | 11.4225 | 0.15696E-04 | 4.4224 | 0.54452E-04 | 26.6401 | 0.30700E-04 |
| 98.78 | 11.4236 | 0.15953E-04 | 4.4238 | 0.56557E-04 | 26.6449 | 0.31446E-04 |
| 104.69 | 11.4247 | 0.16143E-04 | 4.4253 | 0.58621E-04 | 26.6500 | 0.32102E-04 |
| 110.61 | 11.4258 | 0.16274E-04 | 4.4269 | 0.60656E-04 | 26.6551 | 0.32678E-04 |
| 116.53 | 11.4269 | 0.16352E-04 | 4.4285 | 0.62709E-04 | 26.6603 | 0.33191E-04 |
| 122.45 | 11.4280 | 0.16394E-04 | 4.4302 | 0.64843E-04 | 26.6656 | 0.33676E-04 |
| 128.37 | 11.4291 | 0.16354E-04 | 4.4319 | 0.66896E-04 | 26.6709 | 0.34042E-04 |
| 134.29 | 11.4302 | 0.16301E-04 | 4.4337 | 0.69148E-04 | 26.6763 | 0.34433E-04 |
| 140.20 | 11.4313 | 0.16162E-04 | 4.4355 | 0.71323E-04 | 26.6818 | 0.34701E-04 |
| 146.12 | 11.4324 | 0.15980E-04 | 4.4374 | 0.73595E-04 | 26.6873 | 0.34935E-04 |
| 152.04 | 11.4335 | 0.15739E-04 | 4.4394 | 0.75908E-04 | 26.6928 | 0.35105E-04 |
| 157.96 | 11.4345 | 0.15444E-04 | 4.4414 | 0.78324E-04 | 26.6984 | 0.35229E-04 |
| 163.88 | 11.4355 | 0.15109E-04 | 4.4435 | 0.80909E-04 | 26.7040 | 0.35338E-04 |
| 169.80 | 11.4366 | 0.14719E-04 | 4.4457 | 0.83612E-04 | 26.7096 | 0.35403E-04 |
| 175.71 | 11.4375 | 0.14276E-04 | 4.4479 | 0.86490E-04 | 26.7152 | 0.35439E-04 |
| 181.63 | 11.4385 | 0.13748E-04 | 4.4502 | 0.89357E-04 | 26.7208 | 0.35367E-04 |
| 187.55 | 11.4394 | 0.13152E-04 | 4.4526 | 0.92325E-04 | 26.7264 | 0.35232E-04 |
| 193.47 | 11.4403 | 0.12498E-04 | 4.4551 | 0.95518E-04 | 26.7319 | 0.35072E-04 |
| 199.39 | 11.4411 | 0.11770E-04 | 4.4576 | 0.98861E-04 | 26.7374 | 0.34852E-04 |
| 205.31 | 11.4419 | 0.10980E-04 | 4.4603 | 0.10245E-03 | 26.7430 | 0.34606E-04 |
| 211.22 | 11.4426 | 0.10102E-04 | 4.4631 | 0.10614E-03 | 26.7484 | 0.34272E-04 |
| 217.14 | 11.4432 | 0.91352E-05 | 4.4659 | 0.11000E-03 | 26.7538 | 0.33865E-04 |
| 223.06 | 11.4438 | 0.80860E-05 | 4.4689 | 0.11412E-03 | 26.7591 | 0.33409E-04 |

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|---|---|---|---|---|---|---|
| 228.98 | 11.4443 | 0.69500E-05 | 4.4719 | 0.11858E-03 | 26.7644 | 0.32919E-04 |
| 234.90 | 11.4448 | 0.57121E-05 | 4.4751 | 0.12326E-03 | 26.7696 | 0.32347E-04 |
| 240.82 | 11.4451 | 0.43618E-05 | 4.4785 | 0.12816E-03 | 26.7747 | 0.31685E-04 |
| 246.73 | 11.4454 | 0.28992E-05 | 4.4819 | 0.13330E-03 | 26.7796 | 0.30933E-04 |
| 252.65 | 11.4455 | 0.13132E-05 | 4.4855 | 0.13868E-03 | 26.7845 | 0.30081E-04 |
| 258.57 | 11.4455 | -0.40074E-06 | 4.4893 | 0.14448E-03 | 26.7892 | 0.29162E-04 |
| 264.49 | 11.4455 | -0.22639E-05 | 4.4932 | 0.15084E-03 | 26.7937 | 0.28174E-04 |
| 270.41 | 11.4452 | -0.42779E-05 | 4.4973 | 0.15760E-03 | 26.7981 | 0.27085E-04 |
| 276.33 | 11.4449 | -0.64529E-05 | 4.5016 | 0.16459E-03 | 26.8023 | 0.25851E-04 |
| 282.24 | 11.4444 | -0.88104E-05 | 4.5061 | 0.17203E-03 | 26.8063 | 0.24486E-04 |
| 288.16 | 11.4437 | -0.11373E-04 | 4.5108 | 0.18004E-03 | 26.8101 | 0.22991E-04 |
| 294.08 | 11.4428 | -0.14135E-04 | 4.5157 | 0.18889E-03 | 26.8136 | 0.21429E-04 |
| 300.00 | 11.4418 | -0.14124E-04 | 4.5209 | 0.18865E-03 | 26.8169 | 0.21436E-04 |

**IMITON**

Optimized Geometry:

SPACE GROUP (NONCENTROSYMMETRIC) : P 21

11.639314 4.888808 12.813572 90.000 113.731 90.000

| | | | |
|---|---|---|---|
| O | 0.429715 | 0.064314 | 0.068554 |
| O | -0.364205 | -0.239542 | 0.336473 |
| N | -0.325334 | 0.096152 | 0.046893 |
| C | -0.241269 | -0.478307 | -0.496489 |
| C | -0.340696 | 0.114799 | 0.155308 |
| C | -0.457958 | -0.046875 | 0.150246 |
| C | -0.333464 | -0.269540 | 0.449981 |
| C | -0.190352 | 0.365797 | 0.438818 |
| C | -0.203163 | 0.470357 | -0.380182 |
| C | -0.193688 | 0.072916 | 0.061197 |
| C | -0.458447 | -0.049898 | 0.272486 |
| C | -0.106995 | 0.162554 | 0.488531 |
| C | -0.382907 | -0.122954 | -0.487601 |
| C | -0.255477 | -0.371676 | -0.316348 |
| C | -0.341735 | -0.175722 | -0.368644 |
| C | -0.113661 | 0.258829 | -0.329282 |
| C | -0.120643 | 0.339608 | 0.111514 |
| C | -0.068132 | 0.108094 | -0.393086 |
| C | -0.191391 | 0.009896 | -0.056326 |
| H | 0.380330 | -0.090893 | 0.021573 |
| H | -0.375877 | -0.063374 | -0.000990 |
| H | -0.446650 | -0.259484 | 0.129325 |
| H | -0.220321 | 0.414317 | 0.349808 |
| H | -0.147277 | -0.093092 | 0.119712 |
| H | -0.068606 | 0.041185 | 0.439879 |
| H | -0.452576 | 0.032593 | 0.473897 |

H -0.224805 -0.412404 -0.226659
H -0.381573 -0.055434 -0.320713
H -0.084924 0.218611 -0.239561
H -0.002611 -0.055944 -0.355383
H -0.259594 0.031117 0.225739
H -0.350887 0.327223 0.175534
H 0.449438 -0.113348 0.268026
H -0.438539 0.154658 0.310309
H -0.149537 0.500000 0.048068
H -0.020777 0.305695 0.138944
H -0.137876 0.406763 0.184351
H -0.096058 -0.022788 -0.047992
H -0.231361 0.179030 -0.114282
H -0.246623 -0.171531 -0.092483

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THERMAL PROPERTIES FROM HELMHOLTZ FREE ENERGY

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| T (K) | V (Ang^3) | Bt (GPa) | ALPHA (1/K) | Cp-Cv (J/mol*K) | Bs (GPa) | Sp-Sv (J/mol*K) |
|---|---|---|---|---|---|---|
| 10.00 | 686.8096 | 11.224 | 0.36554E-04 | 0.062 | 11.388 | 1.657 |
| 15.92 | 686.9210 | 11.177 | 0.36345E-04 | 0.097 | 11.240 | 4.217 |
| 21.84 | 687.1068 | 11.118 | 0.53285E-04 | 0.285 | 11.212 | 6.490 |
| 27.76 | 687.3503 | 11.053 | 0.66286E-04 | 0.558 | 11.174 | 8.414 |
| 33.67 | 687.6433 | 10.984 | 0.77414E-04 | 0.918 | 11.133 | 10.055 |
| 39.59 | 687.9776 | 10.912 | 0.86414E-04 | 1.337 | 11.088 | 11.479 |
| 45.51 | 688.3450 | 10.840 | 0.93967E-04 | 1.806 | 11.038 | 12.741 |
| 51.43 | 688.7412 | 10.766 | 0.99735E-04 | 2.284 | 10.983 | 13.882 |
| 57.35 | 689.1580 | 10.692 | 0.10583E-03 | 2.850 | 10.932 | 14.932 |
| 63.27 | 689.6038 | 10.617 | 0.11149E-03 | 3.467 | 10.878 | 15.920 |
| 69.18 | 690.0660 | 10.541 | 0.11521E-03 | 4.023 | 10.817 | 16.856 |
| 75.10 | 690.5448 | 10.466 | 0.11917E-03 | 4.642 | 10.758 | 17.752 |
| 81.02 | 691.0401 | 10.391 | 0.12320E-03 | 5.318 | 10.700 | 18.619 |
| 86.94 | 691.5519 | 10.315 | 0.12664E-03 | 5.990 | 10.639 | 19.462 |
| 92.86 | 692.0761 | 10.240 | 0.12945E-03 | 6.641 | 10.576 | 20.285 |
| 98.78 | 692.6126 | 10.165 | 0.13237E-03 | 7.338 | 10.514 | 21.091 |
| 104.69 | 693.1615 | 10.089 | 0.13529E-03 | 8.070 | 10.452 | 21.885 |
| 110.61 | 693.7229 | 10.014 | 0.13800E-03 | 8.813 | 10.389 | 22.670 |
| 116.53 | 694.2965 | 9.939 | 0.14041E-03 | 9.547 | 10.325 | 23.447 |
| 122.45 | 694.8785 | 9.864 | 0.14251E-03 | 10.264 | 10.259 | 24.215 |
| 128.37 | 695.4687 | 9.789 | 0.14459E-03 | 11.002 | 10.194 | 24.976 |
| 134.29 | 696.0672 | 9.715 | 0.14677E-03 | 11.779 | 10.130 | 25.732 |
| 140.20 | 696.6780 | 9.641 | 0.14894E-03 | 12.580 | 10.065 | 26.487 |
| 146.12 | 697.2971 | 9.567 | 0.15091E-03 | 13.369 | 10.000 | 27.238 |
| 152.04 | 697.9245 | 9.493 | 0.15264E-03 | 14.133 | 9.933 | 27.988 |
| 157.96 | 698.5578 | 9.420 | 0.15437E-03 | 14.917 | 9.867 | 28.734 |

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|---|---|---|---|---|---|---|
| 163.88 | 699.1999 | 9.347 | 0.15618E-03 | 15.732 | 9.801 | 29.479 |
| 169.80 | 699.8504 | 9.274 | 0.15789E-03 | 16.546 | 9.735 | 30.225 |
| 175.71 | 700.5095 | 9.202 | 0.15949E-03 | 17.352 | 9.669 | 30.972 |
| 181.63 | 701.1728 | 9.131 | 0.16088E-03 | 18.125 | 9.602 | 31.716 |
| 187.55 | 701.8446 | 9.060 | 0.16246E-03 | 18.954 | 9.536 | 32.461 |
| 193.47 | 702.5206 | 8.989 | 0.16395E-03 | 19.776 | 9.470 | 33.205 |
| 199.39 | 703.2094 | 8.918 | 0.16532E-03 | 20.582 | 9.403 | 33.955 |
| 205.31 | 703.8983 | 8.849 | 0.16679E-03 | 21.425 | 9.338 | 34.700 |
| 211.22 | 704.5956 | 8.780 | 0.16805E-03 | 22.224 | 9.272 | 35.447 |
| 217.14 | 705.3014 | 8.712 | 0.16942E-03 | 23.062 | 9.206 | 36.198 |
| 223.06 | 706.0115 | 8.644 | 0.17067E-03 | 23.880 | 9.141 | 36.949 |
| 228.98 | 706.7258 | 8.577 | 0.17182E-03 | 24.677 | 9.076 | 37.699 |
| 234.90 | 707.4486 | 8.511 | 0.17297E-03 | 25.482 | 9.011 | 38.452 |
| 240.82 | 708.1757 | 8.446 | 0.17421E-03 | 26.324 | 8.947 | 39.206 |
| 246.73 | 708.9070 | 8.382 | 0.17534E-03 | 27.144 | 8.884 | 39.959 |
| 252.65 | 709.6469 | 8.318 | 0.17648E-03 | 27.971 | 8.821 | 40.717 |
| 258.57 | 710.3910 | 8.255 | 0.17771E-03 | 28.839 | 8.759 | 41.474 |
| 264.49 | 711.1393 | 8.194 | 0.17864E-03 | 29.616 | 8.697 | 42.231 |
| 270.41 | 711.8962 | 8.133 | 0.17966E-03 | 30.431 | 8.637 | 42.993 |
| 276.33 | 712.6530 | 8.074 | 0.18068E-03 | 31.256 | 8.577 | 43.751 |
| 282.24 | 713.4183 | 8.016 | 0.18139E-03 | 31.981 | 8.518 | 44.513 |
| 288.16 | 714.1879 | 7.959 | 0.18230E-03 | 32.783 | 8.460 | 45.274 |
| 294.08 | 714.9575 | 7.904 | 0.18298E-03 | 33.510 | 8.403 | 46.033 |
| 300.00 | 715.7357 | 7.850 | 0.18269E-03 | 33.878 | 8.342 | 46.795 |

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LINEAR THERMAL EXPANSION OF CONVENTIONAL LATTICE PARAMETERS

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| T (K) | a (Ang) | ALPHA_a (1/K) | b (Ang) | ALPHA_b (1/K) | c (Ang) | ALPHA_c (1/K) |
|---|---|---|---|---|---|---|
| 10.00 | 11.8377 | 0.22427E-04 | 4.9171 | 0.62444E-05 | 12.8985 | 0.83361E-05 |
| 15.92 | 11.8389 | 0.22301E-04 | 4.9172 | 0.62083E-05 | 12.8989 | 0.82895E-05 |
| 21.84 | 11.8409 | 0.32704E-04 | 4.9174 | 0.90823E-05 | 12.8997 | 0.12156E-04 |
| 27.76 | 11.8435 | 0.40703E-04 | 4.9177 | 0.11254E-04 | 12.9008 | 0.15126E-04 |
| 33.67 | 11.8466 | 0.47562E-04 | 4.9181 | 0.13081E-04 | 12.9020 | 0.17673E-04 |
| 39.59 | 11.8501 | 0.53123E-04 | 4.9185 | 0.14524E-04 | 12.9035 | 0.19737E-04 |
| 45.51 | 11.8540 | 0.57801E-04 | 4.9189 | 0.15700E-04 | 12.9050 | 0.21475E-04 |
| 51.43 | 11.8582 | 0.61388E-04 | 4.9194 | 0.16559E-04 | 12.9067 | 0.22810E-04 |
| 57.35 | 11.8626 | 0.65180E-04 | 4.9199 | 0.17452E-04 | 12.9085 | 0.24223E-04 |
| 63.27 | 11.8673 | 0.68709E-04 | 4.9204 | 0.18257E-04 | 12.9104 | 0.25543E-04 |
| 69.18 | 11.8722 | 0.71040E-04 | 4.9209 | 0.18727E-04 | 12.9124 | 0.26423E-04 |
| 75.10 | 11.8773 | 0.73521E-04 | 4.9215 | 0.19224E-04 | 12.9145 | 0.27363E-04 |
| 81.02 | 11.8826 | 0.76049E-04 | 4.9221 | 0.19720E-04 | 12.9166 | 0.28328E-04 |
| 86.94 | 11.8880 | 0.78208E-04 | 4.9226 | 0.20108E-04 | 12.9188 | 0.29161E-04 |
| 92.86 | 11.8936 | 0.79973E-04 | 4.9232 | 0.20384E-04 | 12.9211 | 0.29859E-04 |
| 98.78 | 11.8993 | 0.81805E-04 | 4.9238 | 0.20670E-04 | 12.9234 | 0.30587E-04 |

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|---|---|---|---|---|---|---|
| 104.69 | 11.9051 | 0.83629E-04 | 4.9244 | 0.20946E-04 | 12.9257 | 0.31320E-04 |
| 110.61 | 11.9110 | 0.85323E-04 | 4.9251 | 0.21183E-04 | 12.9282 | 0.32015E-04 |
| 116.53 | 11.9171 | 0.86823E-04 | 4.9257 | 0.21365E-04 | 12.9307 | 0.32647E-04 |
| 122.45 | 11.9233 | 0.88124E-04 | 4.9263 | 0.21493E-04 | 12.9332 | 0.33215E-04 |
| 128.37 | 11.9296 | 0.89407E-04 | 4.9269 | 0.21612E-04 | 12.9357 | 0.33787E-04 |
| 134.29 | 11.9359 | 0.90742E-04 | 4.9276 | 0.21740E-04 | 12.9383 | 0.34391E-04 |
| 140.20 | 11.9424 | 0.92069E-04 | 4.9282 | 0.21863E-04 | 12.9410 | 0.35004E-04 |
| 146.12 | 11.9490 | 0.93257E-04 | 4.9288 | 0.21950E-04 | 12.9437 | 0.35578E-04 |
| 152.04 | 11.9556 | 0.94281E-04 | 4.9295 | 0.21997E-04 | 12.9465 | 0.36104E-04 |
| 157.96 | 11.9623 | 0.95304E-04 | 4.9301 | 0.22043E-04 | 12.9492 | 0.36643E-04 |
| 163.88 | 11.9691 | 0.96356E-04 | 4.9308 | 0.22094E-04 | 12.9521 | 0.37208E-04 |
| 169.80 | 11.9759 | 0.97344E-04 | 4.9314 | 0.22131E-04 | 12.9549 | 0.37764E-04 |
| 175.71 | 11.9829 | 0.98245E-04 | 4.9321 | 0.22148E-04 | 12.9579 | 0.38303E-04 |
| 181.63 | 11.9899 | 0.99004E-04 | 4.9327 | 0.22135E-04 | 12.9608 | 0.38803E-04 |
| 187.55 | 11.9969 | 0.99864E-04 | 4.9334 | 0.22145E-04 | 12.9638 | 0.39360E-04 |
| 193.47 | 12.0040 | 0.10065E-03 | 4.9340 | 0.22142E-04 | 12.9669 | 0.39907E-04 |
| 199.39 | 12.0113 | 0.10136E-03 | 4.9346 | 0.22123E-04 | 12.9700 | 0.40439E-04 |
| 205.31 | 12.0185 | 0.10211E-03 | 4.9353 | 0.22116E-04 | 12.9731 | 0.41008E-04 |
| 211.22 | 12.0258 | 0.10271E-03 | 4.9359 | 0.22080E-04 | 12.9762 | 0.41538E-04 |
| 217.14 | 12.0331 | 0.10336E-03 | 4.9366 | 0.22061E-04 | 12.9795 | 0.42108E-04 |
| 223.06 | 12.0405 | 0.10393E-03 | 4.9372 | 0.22026E-04 | 12.9827 | 0.42663E-04 |
| 228.98 | 12.0479 | 0.10441E-03 | 4.9379 | 0.21978E-04 | 12.9860 | 0.43206E-04 |
| 234.90 | 12.0554 | 0.10487E-03 | 4.9385 | 0.21932E-04 | 12.9893 | 0.43763E-04 |
| 240.82 | 12.0629 | 0.10538E-03 | 4.9392 | 0.21899E-04 | 12.9927 | 0.44359E-04 |
| 246.73 | 12.0704 | 0.10579E-03 | 4.9398 | 0.21855E-04 | 12.9962 | 0.44942E-04 |
| 252.65 | 12.0780 | 0.10619E-03 | 4.9404 | 0.21813E-04 | 12.9996 | 0.45541E-04 |
| 258.57 | 12.0856 | 0.10663E-03 | 4.9411 | 0.21785E-04 | 13.0032 | 0.46181E-04 |
| 264.49 | 12.0932 | 0.10686E-03 | 4.9417 | 0.21722E-04 | 13.0067 | 0.46757E-04 |
| 270.41 | 12.1009 | 0.10712E-03 | 4.9423 | 0.21675E-04 | 13.0104 | 0.47374E-04 |
| 276.33 | 12.1086 | 0.10736E-03 | 4.9430 | 0.21631E-04 | 13.0140 | 0.48007E-04 |
| 282.24 | 12.1163 | 0.10740E-03 | 4.9436 | 0.21554E-04 | 13.0178 | 0.48574E-04 |
| 288.16 | 12.1240 | 0.10753E-03 | 4.9442 | 0.21506E-04 | 13.0215 | 0.49211E-04 |
| 294.08 | 12.1317 | 0.10751E-03 | 4.9449 | 0.21430E-04 | 13.0253 | 0.49803E-04 |
| 300.00 | 12.1394 | 0.10738E-03 | 4.9455 | 0.21415E-04 | 13.0292 | 0.49760E-04 |