Resolving the structure of $TiBe_{12}$ – Supplementary Material

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Quasi-harmonic thermodynamic data was obtained by repeating the phonon DOS simulation with different unit-cell volumes. The resulting U+F curves (Figure S1) were fitted with a Birch-Murnaghan equation of state [1,2] (Eq. S1).

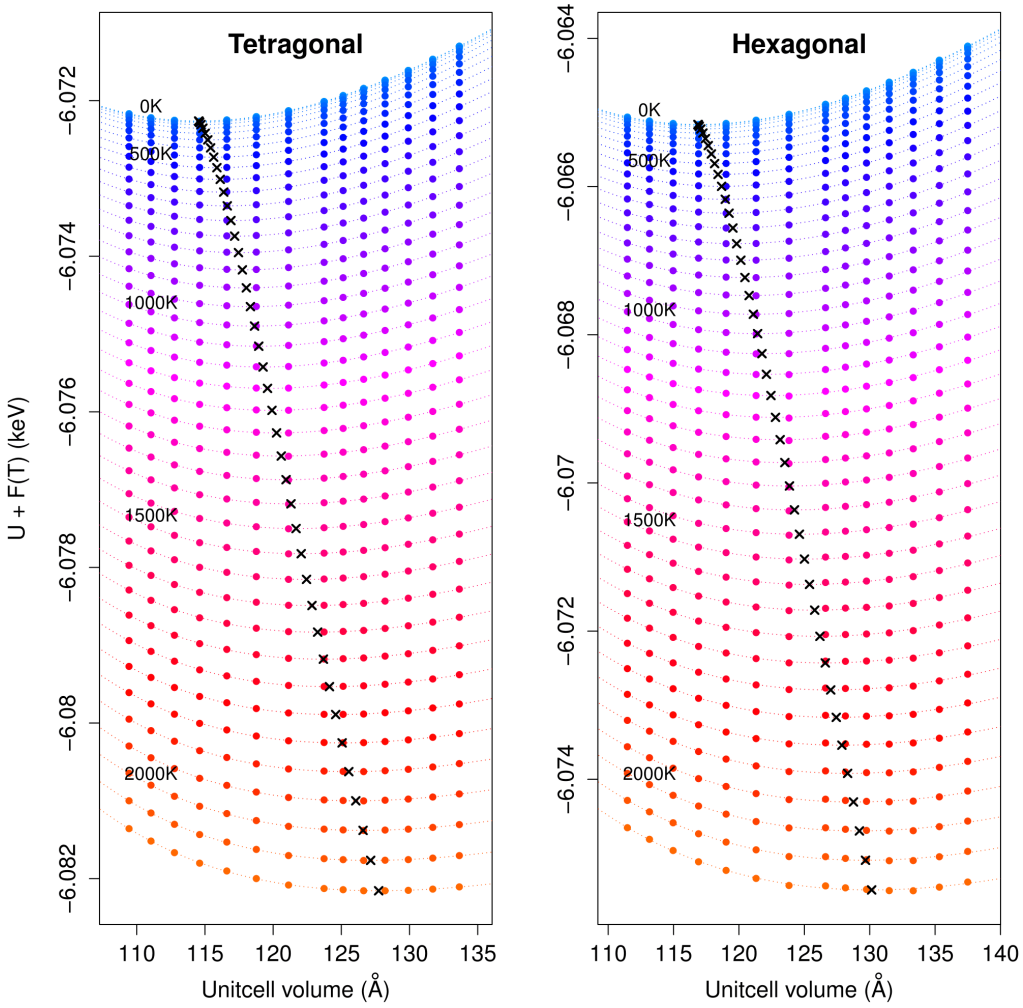

Figure S1 - Thermodynamic data from quasi-harmonic calculations at 50K intervals. Dotted lines are fitted Birch-Murnaghan equations of state, and the crosses represent the minima of those curves.

The Birch-Murnaghan equation (Eq. S1) is represented in the energy-volume form, where E_0 is the ground state energy, V_0 the reference volume, V the deformed volume, K_0 the bulk modulus and K_0' the derivative of the bulk

modulus with respect to pressure. From the minima of the Birch-Murnaghan fits, the volumetric thermal expansion (α_v) was obtained following equation S2.

$$E(V) = E_0 + \frac{9V_0K_0}{16}\left\{\left[\left(\frac{V_0}{V}\right)^{\frac{2}{3}} - 1\right]^3 K_0' + \left[\left(\frac{V_0}{V}\right)^{\frac{2}{3}} - 1\right]^2 \left[6 - 4\left(\frac{V_0}{V}\right)^{\frac{2}{3}}\right]^1\right\} \quad \text{Eq. S1}$$

$$\alpha_V = \frac{1}{V}\frac{dV}{dT} \quad \text{Eq. S2}$$

References

[1] F. Birch, J. Geophys. Res. **83**, 1257 (1978).

[2] F. D. Murnaghan, Proc. Natl. Acad. Sci. U. S. A. **30**, 244 (1944).