Erratum: First-principles prediction of crystal structures at high temperatures using the quasiharmonic approximation [Phys. Rev. B 76, 064116 (2007)]

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Equation (6) had a sign mistyped. It should read

$$\alpha = \frac{1}{V}\left.\frac{\partial V}{\partial T}\right|_{P'}.$$

Equation (9) is the thermodynamic functional relation for F that depends on the two independent variables: $V(P',T')$ and T'. Therefore, Eq. (9) should read

$$F[V(P',T'),T'] = \left\{ U[V(P',T')] + \sum_{\mathbf{q}j} \frac{\hbar\omega_{\mathbf{q}j}[V(P',T')]}{2} \right\} + k_B T' \sum_{\mathbf{q}j} \ln(1 - e^{\hbar\omega_{\mathbf{q}j}[V(P',T')]/k_B T'}).$$

