Electronic Supplementary Material (ESI) for Dalton Transactions

Electronic Supplementary Information:

The expressions for thermodynamic properties of FeSe at high pressure and high temperature

The thermal equation stae $V(P,T)$ can be obtained by solving the non-equilibrium Gibbs function with respect to volume V

$$\left(\frac{\partial G^*(V;P,T)}{\partial V}\right)_{P,T} = 0 \tag{A1}$$

From equation A1, one can get the thermal equation of state. Then, the isothermal bulk modulus B_T, the vibrational internal energy U_{vib}, the heat capacity of constant volume C_V, the heat capacity at constant pressure C_P, the vibrational entropy S_{vib} and the thermal expansion coefficient α can be derived as

$$B_T(P,T) = V\left(\frac{\partial^2 G^*(V;P,T)}{\partial V^2}\right)_{P,T} = 0, \tag{A2}$$

$$U_{vib} = nk\left[\frac{9}{8}\frac{\Theta}{T} + 3D(3\Theta/T)\right], \tag{A3}$$

$$C_V = 3nk\left[4D(\frac{\Theta}{T}) - \frac{3\Theta/T}{e^{\Theta/T}-1}\right], \tag{A4}$$

$$C_P = C_V(1+\alpha\gamma T), \tag{A5}$$

$$S_{vib} = nk\left[4D(3\Theta/T) - 3\ln(1-e^{-\Theta/T})\right], \tag{A6}$$

$$\alpha = \frac{\gamma C_V}{B_T V}, \tag{A7}$$

where the Grüneisen parameter γ is defined as

$$\gamma = -\frac{d\ln\Theta(V)}{\ln V} \tag{A8}$$