Errata in this article:

MHG Jacobs, TU-Clausthal, June 21st, 2013. Last update November 30th 2014

Refers to:
Jacobs MHG, Schmid-Fetzer R, van den Berg AP (2013) An alternative use of Kieffer's lattice dynamics model using vibrational density of states for constructing thermodynamic databases. *Phys Chem Minerals* **40**:207-227

1. January 27th, 2014, Helmholtz energy
Equation (12), p222 for the anharmonic contribution to Helmholtz energy has a misprint. The correction has been marked by the red circle:

$$A_{anh}^{vib} = 3nRT^2 \sum_{j=1}^{N_E} \frac{a_j}{6} f_j \left[\frac{1}{4} \left(\frac{\theta_j^E}{T} \right)^{\textcircled{2}} + \frac{3 \left(\theta_j^E / T \right)^2 \exp\left(\theta_j^E / T \right)}{\left(\exp\left(\theta_j^E / T \right) - 1 \right)^2} \right] \tag{12}$$

2. June 21st 2013, isothermal bulk modulus
Equation (32), p225 in the appendix, containing the anharmonic contribution to isothermal bulk modulus has a misprint. The correction has been marked by the red circle in the equation below.

Anharmonic contribution to isothermal bulk modulus

$$K_{anh}^{vib} = \frac{3nRT^2}{V} \sum_{j=1}^{N_E} \frac{a_j}{6} f_j \left[\gamma_j - V \left(\frac{\partial \gamma_j}{\partial V} \right)_T \right] \left[\frac{x_j^2}{2} + \frac{3x_j^2 (2 - x_j) e^{2x_j} - 3x_j^2 (2 + x_j) e^{x_j}}{\left(e^{x_j} - 1 \right)^3} \right] +$$

$$+ \frac{3nRT^2}{V} \sum_{j=1}^{N_E} \frac{a_j \gamma_j^2}{6} f_j \left[x_j^2 + \frac{e^{3x_j} (12x_j^2 - 15x_j^3 + 3x_j^4) + e^{2x_j} (-24x_j^2 + 12x_j^4) + e^{x_j} (12x_j^2 + 15x_j^3 + 3x_j^4)}{\left(e^{x_j} - 1 \right)^4} \right] +$$

$$+ 3nRT^2 V \sum_{j=1}^{N_E} \frac{a_j''}{6} f_j \left[\frac{\textcircled{x_j^2}}{4} + \frac{3x_j^2 e^{x_j}}{\left(e^{x_j} - 1 \right)^2} \right] +$$

$$- 3nRT^2 \sum_{j=1}^{N_E} \frac{a_j' \gamma_j}{6} f_j \left[\frac{x_j^2}{2} + \frac{3x_j^2 (2 - x_j) e^{2x_j} - 3x_j^2 (2 + x_j) e^{x_j}}{\left(e^{x_j} - 1 \right)^3} \right] \tag{32}$$

3. June 21st, 2013, electronic heat capacity
There is a mistake in the expression for the electronic contribution for platinum in Table 4, page 216. It should read as:

$$C_V^{el,el-ph} = \left\{ \sum_{i=1}^{3} a_i T^i e^{-b_i T} + c_1 T + c_2 \left(1 - \frac{1}{c_3 T + 1} \right) \right\} \left(\frac{V}{V_0} \right)^{\gamma_{el}}$$ (Table 4, p216)

4. November 30th 2014, Figure 5
Unit must be cm^3/0.5mol.