Murnaghan fit

$$E = \underset{\substack{\uparrow \\ p_1}}{x(1)} + \underset{\substack{\uparrow \\ p_2}}{x(3)} \cdot V \cdot \frac{1}{\underset{\substack{\uparrow \\ p_3}}{x(4)}\left[x(4)-1\right]} \left\{ x(4)\left[1-\frac{\overset{\substack{p_4 \\ \downarrow}}{x(2)}}{V}\right] + \left(\frac{x(2)}{V}\right)^{x(4)} - 1 \right\}$$

$$\frac{\partial E}{\partial V} = \frac{p_2}{p_3}\left[1-\left(\frac{p_4}{V}\right)^{p_3}\right] \; ; \quad \frac{\partial E}{\partial V} = 0 \;\Rightarrow\; \boxed{p_4 = V_{eq.}}$$

$$\frac{\partial^2 E}{\partial V^2} = \frac{p_2}{V}\left(\frac{p_4}{V}\right)^{p_3}$$

$$B = p_2\left(\frac{p_4}{V}\right)^{p_3} \; ; \quad \frac{\partial E}{\partial V} = 0 \;\Rightarrow \qquad \boxed{p_2 = B\,.}$$

$$P = -\frac{p_2}{p_3}\left[1-\left(\frac{p_4}{V}\right)^{p_3}\right] \; ; \quad P = -\frac{p_2}{p_3} + \frac{1}{p_3} B \; ;$$

$$B = p_2 + p_3 P \; ; \qquad \boxed{B' \equiv \frac{\partial B}{\partial P} = p_3}$$

$$\boxed{E(V_{eq.}) = p_1}$$

Conversion: p_2 from the fit is in $\left[\frac{Ry}{(a.u.)^3}\right]$;

$$B = -V\frac{\partial P}{\partial V} = V\frac{d^2 E}{dV^2}$$

Conversion: p_2 from the fit is in $\left[\frac{Ry}{(a.u.)^3}\right]$;

$$1\ \frac{Ry}{(a.u.)^3} = \frac{\overbrace{13.61}^{eV/Ry} \times \overbrace{1.60219 \cdot 10^{-19}}^{J/eV}\ J}{\underbrace{0.529177}_{Å/a.u.}{}^{3} \cdot 10^{-30}\ m^3} =$$

$$= \underbrace{\frac{13.61 \times 1.60219}{0.529177^3} \cdot 100 \cdot 10^9}\ \frac{N}{m^2} =$$

$$= 14715.3\ GPa$$

$$= 147153\ KBar$$

Exp. values of B at room temperature:

Fe	1683 kBar →	
Mn	596	
Al	722	
Cu	1370	
Ni	1860	
Ti	1051	

calculation for Fe:

2097 (TBLMTO)
2166 (WIEN-LDA)
1699 (WIEN-GGA)

1 bar = 10^5 Pa
1 kbar = 0,1 GPa