Using the identity,

$$V = \left(\frac{\partial G}{\partial P}\right)_T , \qquad (A.13)$$

and combining Eqs. (A.2), (A.8), (A.9), (A.12), and (A.13) results in

$$\left(\frac{\partial f(V)}{\partial V}\right)_T = - T_0 \, b \, C_V + B_0 \, V_0 \left[\left(\frac{V}{V_0}\right)^{-1} - 1\right] . \qquad (A.14)$$

Integrating Eq. (A.14) for $f(V)$ and substituting in Eq. (A.2) results in the expression,

$$E = E_0 + C_V(T-T_0) - T_0 \, b \, C_V(V_0-V) + V_0 \, B_0 \left[\frac{\left(\frac{V}{V_0}\right)^{1-n} - 1}{n-1} - \frac{V_0-V}{V_0}\right] . \qquad (A.15)$$

Equations (A.8), (A.12), and (A.15) define the phase 1 and phase 2 equilibrium surfaces within initial values V_{01}, V_{02}, E_{01}, E_{02}, S_{01}, and S_{02}. The value for V_{01} for iron is easily measured while V_{02} has been inferred from x-ray measurements of coexisting phases.[33] The value for S_{01} can be arbitrarily chosen while S_{02} is fixed by the difference in entropy between phases which can be inferred from the measured slope of the phase line or obtained from a thermodynamically consistent empirical equation of state which is fitted to all types of experimental data.[27,28] The magnitude of E_{01} can be arbitrarily chosen while E_{02} must be specified by some additional relationship. A relationship which makes the connection between the equilibrium surfaces is:

$$G_{21}(P^*,T^*) = 0 , \tag{A.16}$$

where G_{21} is the difference between Gibbs energies of the phases, (P^*,T^*) is the equilibrium transformation point. This equilibrium condition with Eq. (A.9) determines the value of E_{02}. Use of Eq. (A.16) to determine the equilibrium surface provides no assurance that the state point in any real process will actually lie on such a surface (cf Chapter 5).

The values for E_{01}, S_{01}, and S_{02} at 1 atmosphere pressure and a temperature of 295°K were chosen to be the same as those used by Andrews.[27,28] The value for E_{02} was determined from the relation G_{21}(116 kbar,332°K) = 0. The initial value of C_{V2} is the classical value of $3R$ where R is the gas constant. The initial values used to define the equilibrium surfaces are listed in Table A.1.

TABLE A.1.--Initial values
(T=295°K,P=0)

Variable	Alpha phase	Epsilon phase
V_0	0.1272	0.1208 cm^3/gm
E_0	7.932×10^{-4}	1.667×10^{-3} Mbar cm^3/gm
S_0	4.863×10^{-6}	5.323×10^{-6} Mbar cm^3/gm deg
n	5.917	5.102
B_0	0.275	0.325 Mbar
Γ	1.735	2.0
C_V	4.447×10^{-6}	4.466×10^{-6} Mbar cm^3/gm deg