

Supplementary material. First-order transition at constant volume: a continuous transition?

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The first-order phase transition between liquid and ice-VI water phases is driven under isochoric condition ($V_0 = 13.4 \text{ cm}^3/\text{mol}$). Figures [S1](#), [S2](#) and [S3](#) show the corresponding changes in the Gibbs energy $\Delta G(T) = G(T) - G_m^{liq}(T_1)$, the internal energy $\Delta U(T) = U(T) - U_m^{liq}(T_1)$ and the enthalpy $\Delta H(T) = H(T) - H_m^{liq}(T_1)$, respectively. As predicted, all of them are continuous at T_1 and T_2 , the temperature onset and end of the transition, respectively.

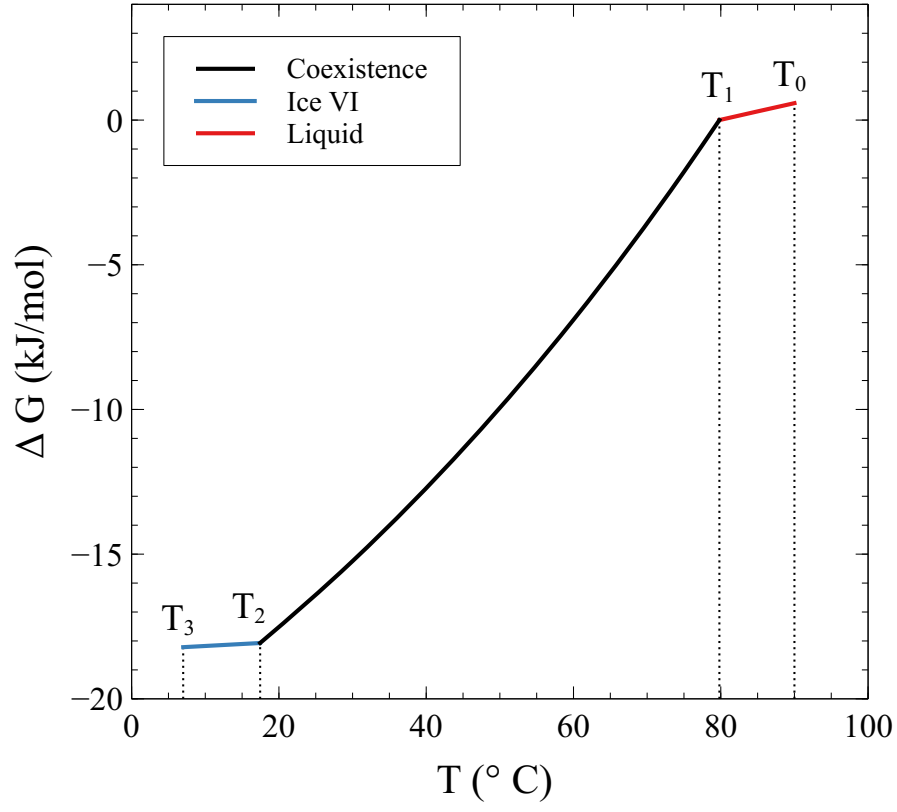


Figure S1: The Gibbs energy change $\Delta G(T) = G(T) - G_m^{liq}(T_1)$ in a process at constant volume $V_0 = 13.4 \text{ cm}^3/\text{mol}$.

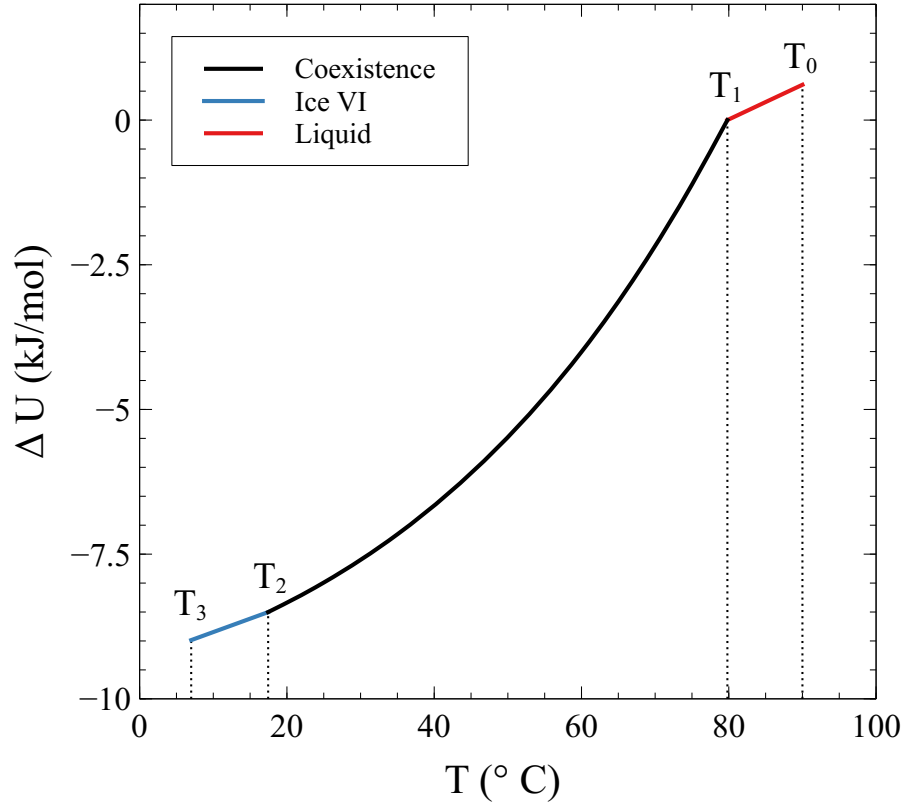


Figure S2: The internal energy change $\Delta U(T) = U(T) - U_m^{liq}(T_1)$ in a process at constant volume $V_0 = 13.4 \text{ cm}^3/\text{mol}$.

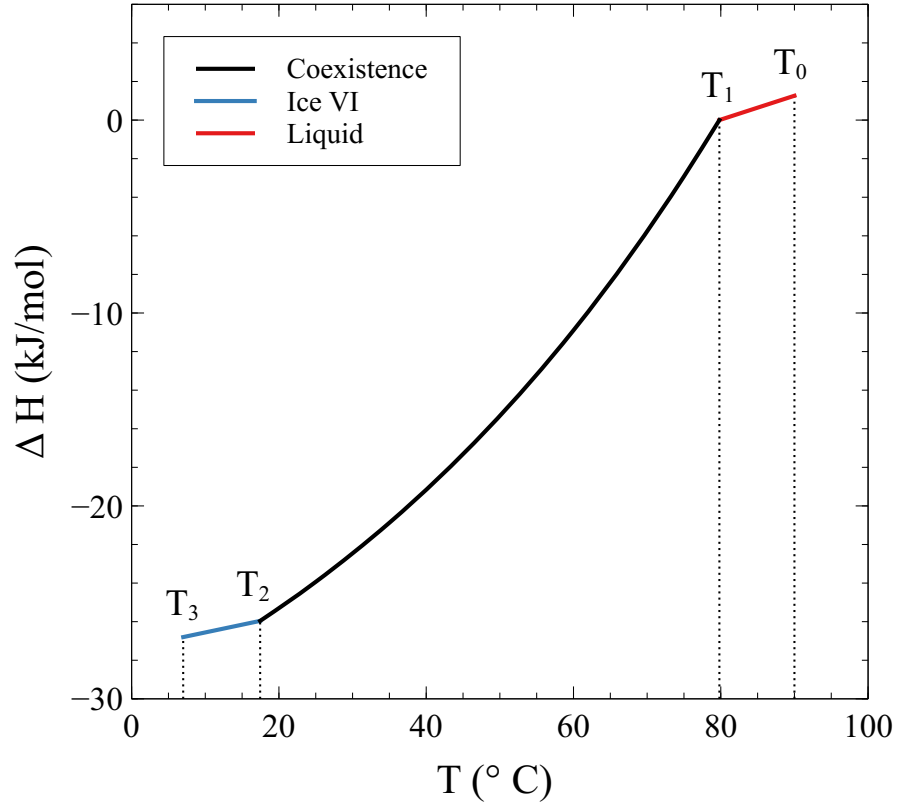


Figure S3: The enthalpy change $\Delta H(T) = H(T) - H_m^{liq}(T_1)$ in a process at constant volume $V_0 = 13.4$ cm³/mol.