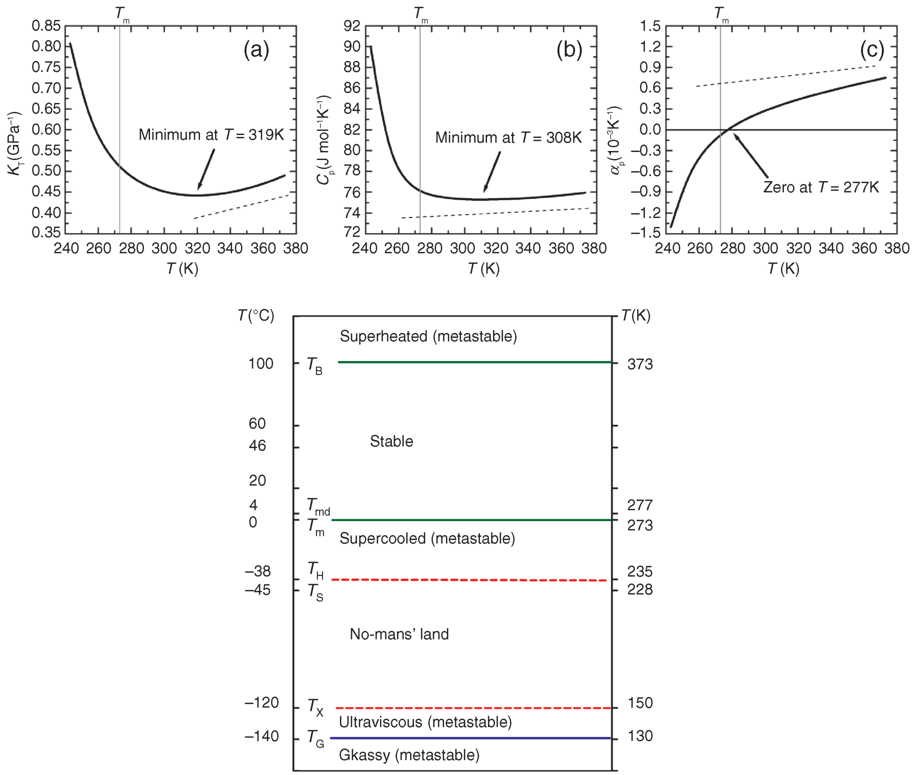

Figure 10.1. Examples of water's thermodynamic anomalies. Dependence on temperature of **(a)** the isothermal compressibility K_T, **(b)** the isobaric specific heat C_p, and **(c)** the coefficient of thermal expansion α_p. The behavior of water is indicated by the solid line; that of a typical liquid by the dashed line. Data from Ref. [5]. Bottom: Schematic illustration of different temperature domains, at atmospheric pressure, of H_2O. Only one domain is stable; the others are metastable.

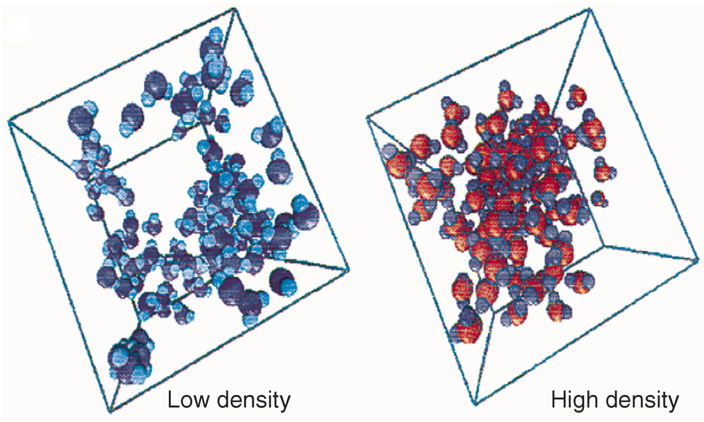

Figure 10.3. Molecular dynamics snapshots of LDL and HDL, coexisting and separating in liquid water [3].

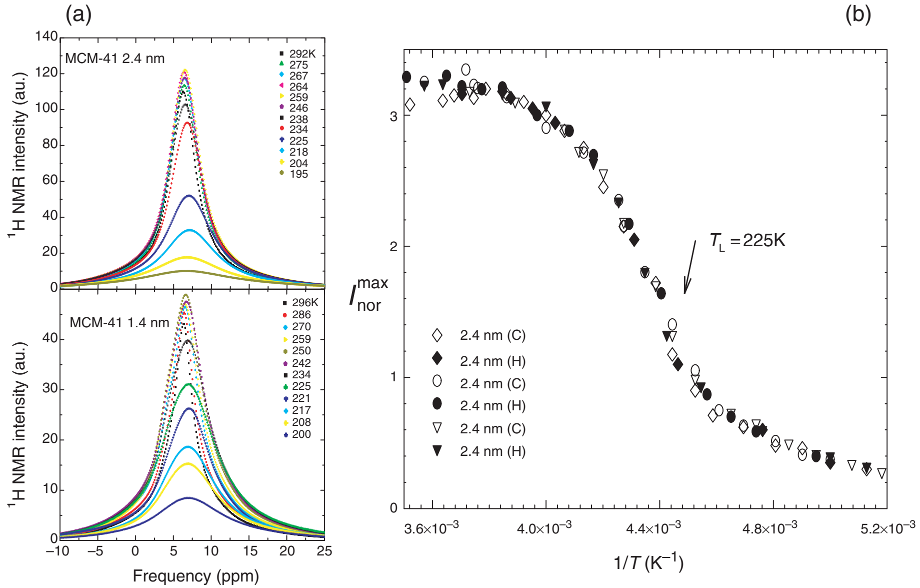

Figure 10.6. (a) The ^{1}H NMR spectra of water in MCM samples with $\phi = 24$ and 14 Å, upon cooling. (b) The normalized NMR intensities, $I_{\mathrm{Nor}}^{\max}$ versus $1/T$, for $\phi = 14$, 18, and 24 Å samples [75].

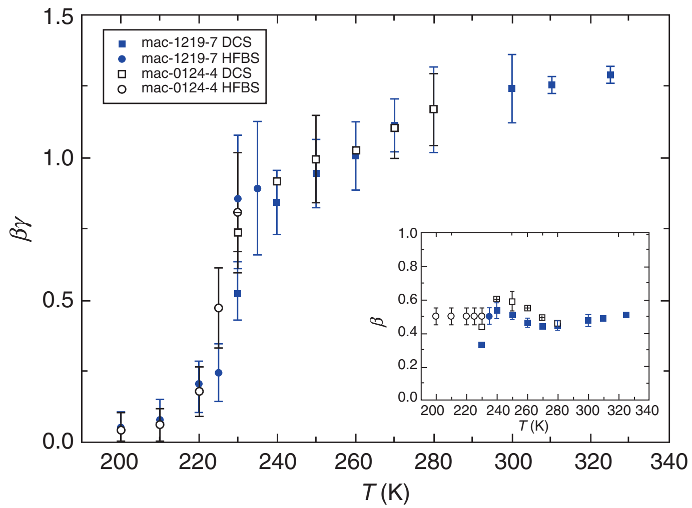

Figure 10.7. Temperature dependence of $\beta\gamma$, which is the exponent expressing the Q-dependence of the translational ISF for the MCM sample. Note that the figure shows a sharp break at $\approx$ 225K. The inset reports the T-dependence of the exponent β [98].

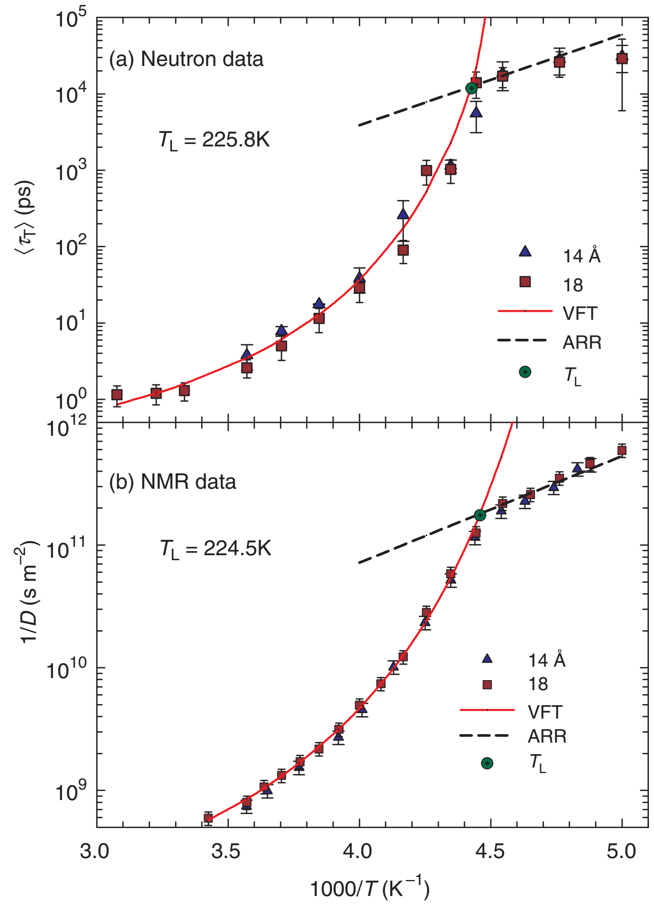

Figure 10.9. The ambient pressure values of the $\langle \tau_T \rangle$ (a—QENS) and of the $1/D$ (b—NMR) as a function of $1/T$ in fully hydrated MCM-41-S.

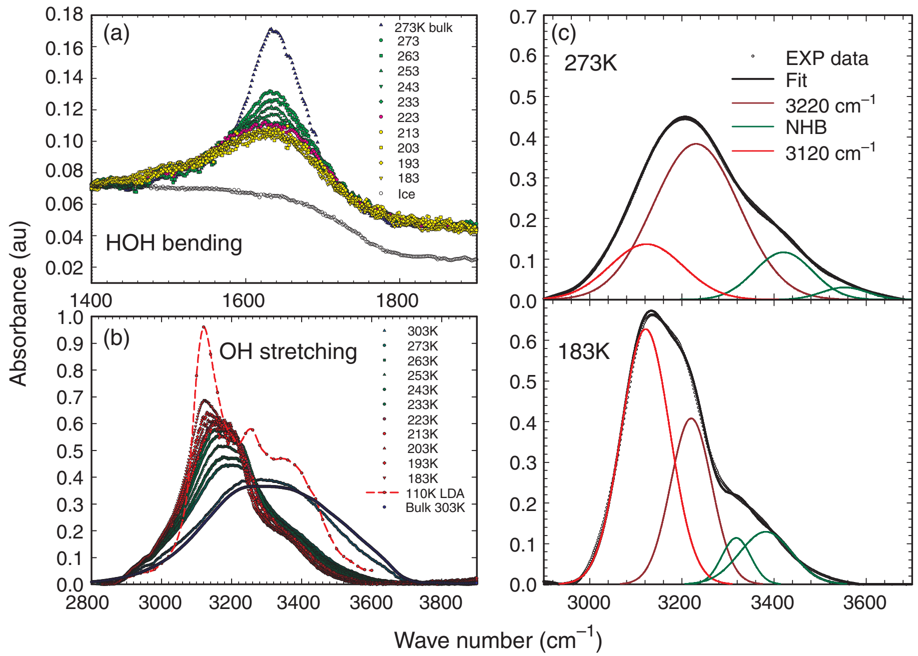

Figure 10.11. **(a)** The HOH bending and **(b)** the O–H stretching vibrational spectra of MCM confined water at the different temperatures [88]. **(c)** Examples of the spectral fitting results.

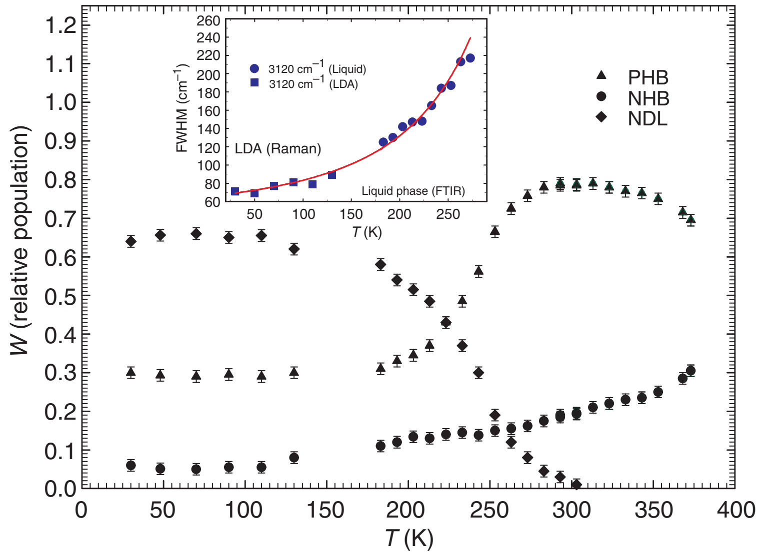

Figure 10.12. The FWHM values of the OH stretching spectral component I (3120 cm^{-1}) versus T, measured in confined water and in the LDA phase [88,105] (inset). T-dependence of the fractioned relative populations of the LDL, W_{LDL} (diamonds), and of the HDL, W_{HDL} (triangles and circles) water phases [106].

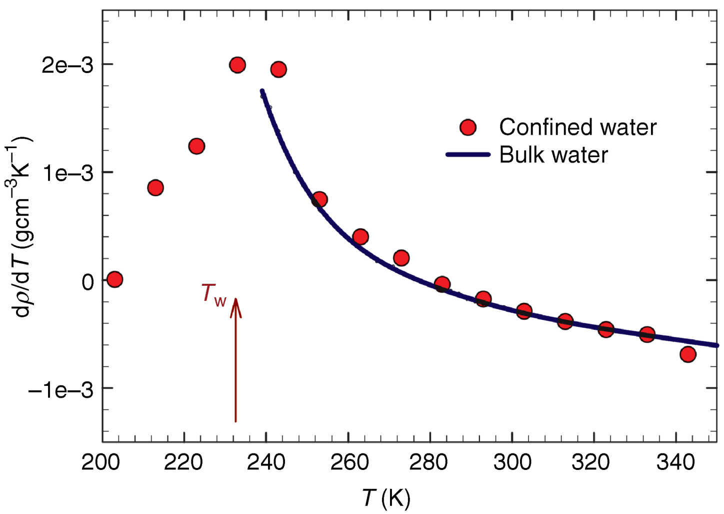

Figure 10.14. The density derivative $(\partial\rho/\partial T)_p$. The arrow indicates the Widom temperature T_W. $(\partial\rho/\partial T)_p$, related with the cross-correlation between the entropy and volume fluctuations, is proportional to the thermal expansion coefficient [106].

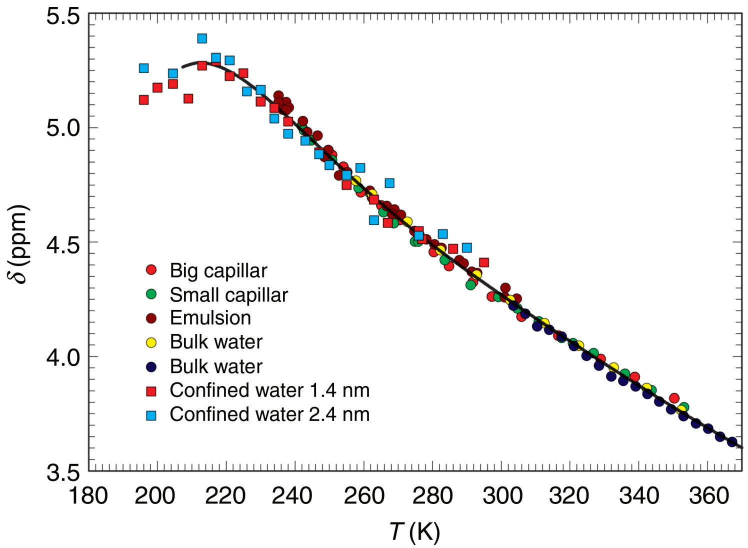

Figure 10.24. The temperature behavior of the water proton chemical shift δ. Our data (squares) and data from the literature (circles) [133].

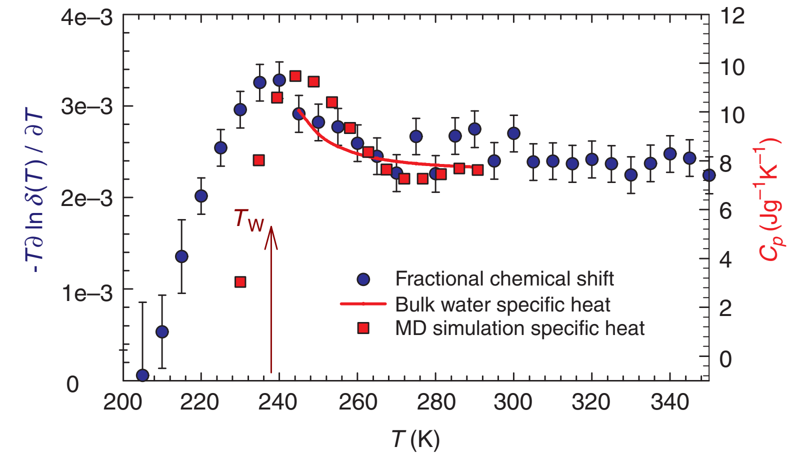

Figure 10.25. The temperature derivative of the measured fractional chemical shift $-T\partial \ln \delta(T)/\partial T$ (blue circles, left-hand side), the specific heat at constant pressure, C_p (right-hand side), measured in bulk water in the supercooled regime (red line, Ref. [124]), and C_p calculated for the TIP5P model of water (red squares, Ref. [143]).