Key Homework 4

$$\frac{C_{v,vib}}{R} = \sum_{j=1}^{\infty}\left[\left(\frac{\Theta_{vib,j}}{T}\right)^2 \frac{e^{-\Theta_{vib,j}/T}}{\left(1-e^{-\Theta_{vib,j}/T}\right)^2}\right] \quad \text{Eq 18.48}$$

each term of sum represents contribution from each normal mode

$\Theta_{vib}^{H_2O} = 5360\ K\ (1),\ 5160\ K\ (2),\ 2290\ K\ (3)$ · $T = 600\ K$

① $\frac{C_v}{R} = \left(\frac{5360}{600}\right)^2 \frac{e^{-5360/600}}{\left(1-e^{-5360/600}\right)^2} = 1.05 \times 10^{-2}$

② $C_v/R = 1.36 \times 10^{-2}$

③ $C_v/R = 0.335$ largest contribution... from below - this the bending mode

C_v/R total = 0.359

NIST

Symmetric stretch	3657 cm^{-1}	$\Theta_{vib} = \frac{h\nu}{k_B} = \frac{hc\tilde{\nu}}{k_B}$
bend	1595 cm^{-1}	$\Theta_{vib} = 5267.7\ K \sim$ ②
antisymetric stretch	3756 cm^{-1}	$\Theta_{vib} = 2297.5\ K \sim$ ③
		$\Theta_{vib} = 5410.3\ K \sim$ ①