HEAT CAPACITY OF A SINGLE WATER MOLECULE

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Reference: Daniel V. Schroeder, An Introduction to Thermal Physics, (Addison-Wesley, 2000) - Problem 1.43.
The specific heat capacity of water is $1 \text{ cal g}^{-1} \text{°C}^{-1} = 4.186 \text{ J g}^{-1} \text{°C}^{-1}$, so how does this translate into the heat capacity per water molecule? The molar weight of water is $18.01528 \text{ g mol}^{-1}$ so in 1 gram of water there are

$$N = \frac{6.02 \times 10^{23}}{18.01528} = 3.3416 \times 10^{22} \text{ molecules} \quad (1)$$

The heat capacity of a single molecule is therefore

$$C = \frac{4.186}{3.3416 \times 10^{22}} = 1.2527 \times 10^{-22} \text{ J °C}^{-1} \quad (2)$$

$$= 9.08k \quad (3)$$

where $k$ is Boltzmann’s constant.

Thus to raise the temperature of a sample of water by 1° C, we need to raise the energy of each molecule by around $9k$. If we assumed that all the thermal energy of water is due to quadratic degrees of freedom, then because each degree of freedom contributes $\frac{1}{2}kT$ to the energy, we would need 18 degrees of freedom in a water molecule. As we’ve seen, water has around 10 such degrees of freedom, so the thermal energy must also be stored elsewhere.