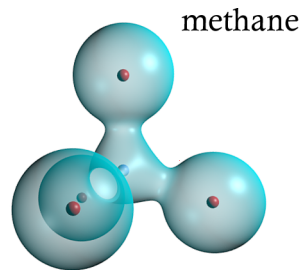


Thermodynamics - Equipartition theorem - Internal molecular degrees of freedom relax

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Ok, you are given a methane molecule alone. Find the total energy of this single molecule at the temperature $T = 300\text{K}$.



There are 16 DOF(degree of freedom).

Count	D.O.F.	Meaning	Energy
1	mv_x	Linear momentum in x	$\frac{1}{2}mv_x^2$
2	mv_y	Linear momentum in y	$\frac{1}{2}mv_y^2$
3	mv_z	Linear momentum in z	$\frac{1}{2}mv_z^2$
4	$I\omega_x$	Angular momentum around x	$\frac{1}{2}I\omega_x^2$
5	$I\omega_y$	Angular momentum around y	$\frac{1}{2}I\omega_y^2$
6	$I\omega_z$	Angular momentum around z	$\frac{1}{2}I\omega_z^2$
7	n_{s1}	Strech vibration mode 1	$\hbar\omega_s$
8	n_{s2}	Strech vibration mode 2	$\hbar\omega_s$
9	n_{s3}	Strech vibration mode 3	$\hbar\omega_s$
10	n_{s4}	Strech vibration mode 4	$\hbar\omega_s$
11	n_{b1}	Bend vibration mode 1	$\hbar\omega_b$
12	n_{b2}	Bend vibration mode 2	$\hbar\omega_b$
13	n_{b3}	Bend vibration mode 3	$\hbar\omega_b$
14	n_{b4}	Bend vibration mode 4	$\hbar\omega_b$
15	n_{b5}	Bend vibration mode 5	$\hbar\omega_b$
16	n_{b6}	Bend vibration mode 6	$\hbar\omega_b$

The equipartition theorem tells us that each degree of freedom gets $\frac{1}{2}kT$, so assuming maximal entropy the molecule has a total internal energy of $8kT$. So the total energy at 300K is,

$$E_{\text{tot}} = 8 \cdot \left(1.38 \cdot 10^{-23} \frac{\text{m}^2\text{kg}}{\text{s}^2\text{K}} \right) \cdot 300\text{K} \simeq 3.3 \cdot 10^{-20} \text{J}$$