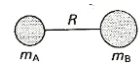
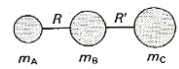
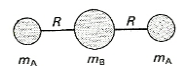
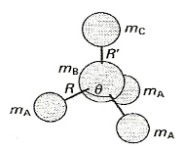
Appendix 2

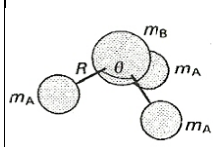
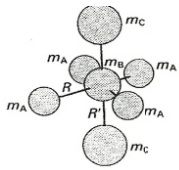
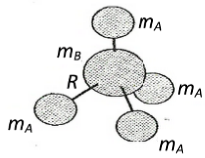
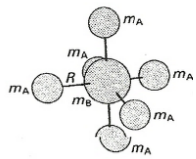
Moments of Inertia of Molecules

In the tables below, we find the expressions of moments of inertia for several common forms of molecules.

m is the total mass of molecule, m_A is the mass of atom A.

Rotor	Form	I
Diatomic molecules		$\frac{m_A m_B}{m_A + m_B} R^2$
Linear rotor		$m_A R^2 + m_C R'^2 - \frac{(m_A R - m_C R')^2}{m}$
Linear rotor		$2m_A R^2$
Symmetrical rotor		$I_{II} = 2m_A R^2 (1-\cos\theta)$ $I_{=} = m_A R^2 (1-\cos\theta)$ $+\frac{m_A}{m}(m_A + m_C)R^2(1+2\cos\theta)$ $+\frac{m_C R'^2}{m}\left\{\begin{array}{l}(3m_A + m_B)R' + \\ 6m_A R\left[\frac{1}{3}(1+2\cos\theta)\right]^{1/2}\end{array}\right\}$

Phase Modeling Tools: *Applications to Gases*, First Edition. Michel Soustelle.

Rotor	Form	I
Symmetrical rotor		$I_{\mathrm{II}} = 2m_{\mathrm{A}}R^2(1-\cos\theta)$ $\mathrm{I}_{\perp} = m_{\mathrm{A}}R^2(1-\cos\theta)$ $+\frac{m_{\mathrm{A}}m_{\mathrm{B}}}{m}R^2(1+2\cos\theta)$
Symmetrical rotor		$I_{\mathrm{II}} = 4m_{\mathrm{A}}R^2$ $\mathrm{I}_{\perp} = 2m_{\mathrm{A}}R^2 + 2m_{\mathrm{C}}R'^2$
Spherical rotor		$\frac{8}{3}m_{\mathrm{A}}R^2$
Spherical rotor		$4m_{\mathrm{A}}R^2$