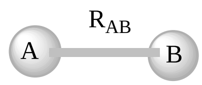
Moments of Inertia of Common Molecules

Linear

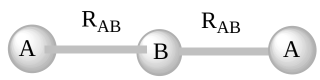
Diatomic $I_c = I_b > I_a = 0$

$$I = \frac{m_A m_B}{m_A + m_B} R_{AB}^2$$



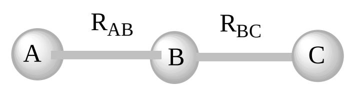
Symmetric Triatomic

$$I = 2m_A R_{AB}^2$$



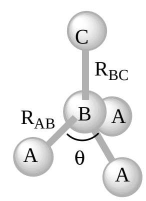
Non-symmetric Triatomic

$$I = m_A R_{AB}^2 + m_C R_{BC}^2 - \frac{(m_A R_{AB} - m_C R_{BC})^2}{m_A + m_B + m_C}$$



Symmetric Rotors $I_c = I_b > I_a$ (Prolate symmetric rotor)
$I_c > I_b = I_a$ (Oblate symmetric rotor)

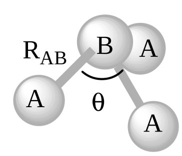
Type A_3BC



$$I_a = 2m_A R_{AB}^2 (1 - \cos\theta)$$

$$I_c = m_A R_{AB}^2 (1 - \cos\theta) + \frac{m_A}{\sum m_i}(m_B + m_C) R_{AB}^2 (1 + 2\cos\theta) + \frac{m_C R_{BC}^2}{\sum m_i}\left\{(3m_A + m_B) R_{BC} + 6 m_A R_{AB}\left[\frac{1}{3}(1 + 2\cos\theta)\right]^{1/2}\right\}$$

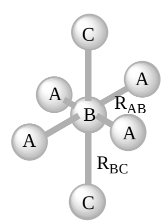
Type A_3B



$$I_a = 2m_A R_{AB}^2 (1 - \cos\theta)$$

$$I_c = m_A R_{AB}^2 (1 - \cos\theta) + \frac{m_A m_B}{\sum m_i} R_{AB}^2 (1 + 2\cos\theta)$$

Type A_4BC_2



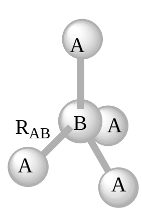
$$I_a = 4m_A R_{AB}^2$$

$$I_c = 2m_A R_{AB}^2 + 2m_C R_{BC}^2$$

Spherical Rotors $I_c = I_b = I_a$

Tetrahedral

$$I = \frac{8}{3} m_A R_{AB}^2$$



Octahedral

$$I = 4m_A R_{AB}^2$$