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The Tensor of the Moment of Inertia

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I. SYNOPSIS

For polyatomic molecules, the moment of inertia, a tensor, is needed in order to study its dynamics and quantum mechanics.

II. DIATOMICS

The moment of inertia is computed relative to the center of mass, which for a diatomic molecule is easy to picture, it is the place where the "see-saw" balances, i.e., where the clockwise and counter clockwise torques balance each other out. We then have (see figure 1)

$$m_A r_A = m_B r_B \tag{2.1}$$

as the condition for torque balance ("see-saw" equilibrium). Further, defining the internuclear distance as R, we have

$$R = r_A + r_B$$

Clearly

$$R^2 = r_A^2 + 2r_a r_B + r_B^2 \tag{2.2}$$

and, from Equation 2.1

$$0 = m_A^2 r_A^2 - 2m_A m_B r_A r_B + m_B^2 r_B^2 \tag{2.3}$$

so, multiplying Equation 2.2 by $m_A m_B$ one has, upon adding the resultant to Equation 2.3,

$$m_A m_B R^2 = m_A m_B r_A^2 + m_A m_B r_B^2 + m_A^2 r_A^2 + m_B^2 r_B^2$$

which we rewrite as

$$m_A m_B R^2 = m_A(m_B + m_A) r_A^2 + m_B(m_A + m_B) r_B^2$$

and since

$$\frac{1}{\mu} = \frac{1}{m_A} + \frac{1}{m_B}$$

we have

$$\mu = \frac{m_A m_B}{m_A + m_B}$$

which leads us to

$$\mu R^2 = m_A r_A^2 + m_B r_B^2 = I$$

i.e., we have obtained a pseudo particle (of mass μ) moment of inertia which mimics the two particle value. Said another way, when one is sitting on the center of mass of a two particle central force problem situation, then the moment of inertia of that two body system is identical in all respects to the moment of inertia of a single particle whose mass is the reduced mass, and whose separation from the origin is exactly equal to the sum of the two moment arms which separated the bodies in the first place.

III. POLYATOMICS

For an arbitrary molecule, we define a local coördinate system in whatever method seems simplest, and calculate the center of mass for that coördinate system. Next, we translate ourselves to that center of mass. From here on in, we assume that we are on the center of mass!

Next, we define the tensor of the moment of inertia as

$$\begin{pmatrix} I_{xx} & I_{xy} & I_{xz} \\ I_{xy} & I_{yy} & I_{yz} \\ I_{zx} & I_{zy} & I_{zz} \end{pmatrix}$$

where, summing over all nuclei, we have

$$I_{xx} = \sum_i m_i(y_i^2 + z_i^2)$$

$$I_{yy} = \sum_i m_i(x_i^2 + z_i^2)$$

$$I_{zz} = \sum_i m_i(x_i^2 + y_i^2)$$

and

$$I_{xy} = \sum_i m_i(x_i y_i)$$

$$I_{xz} = \sum_i m_i(x_i z_i)$$

$$I_{yz} = \sum_i m_i(z_i y_i)$$

Now we need a molecule. Consider water. The O-H bond length in water is 0.9584Å. The H-O-H bond angle is 104.5^o. We will place the oxygen atom on the y-axis, and work in the x-y plane, i.e., the center of mass is on

the H-O-H angle bisector, between the average proton position and the oxygen. Technically,

$$m_O|y_O| = 2m_H|y_H|$$

defines the center of mass but

$$\cos\frac{\theta}{2} = \frac{y_O - y_H}{r_{OH}}$$

so

$$m_O y_O = 2m_H\,(y_O - r_{OH}\cos\theta/2)$$

remembering that the protons lie at negative y values. We obtain

$$16y_O = 2(y_O - 0.9584 \times 0.6122) = 2(y_O - 0.586749)$$

or

$$y_O = \frac{0.586749}{14} = 0.04191$$

Then

$$x_H = \pm 0.9584 \sin\frac{104.5}{2} = \pm 0.7578$$

and

$$y_H = +0.58675 - 0.04191 = -0.54484$$

Atom	x	y	z
O	0	0.0652	0
H_1	0.7578	-0.54484	0
H_2	-0.7578	-0.54484	0

Continuing, we have

$$I_{xx} = \sum_i m_i(y_i^2 + z_i^2) = m_O(0.0652 \times 10^{-8})^2 + 2m_H(0.5425 \times 10^{-8})^2$$

$$I_{zz} = \sum_i m_i(x_i^2 + y_i^2) = m_O(0.0652 \times 10^{-8})^2 + 2m_H[(0.5425 \times 10^{-8})^2 + (0.7578 \times 10^{-8})^2] = 3.00 \times 10^{-40}$$

$$I_{yy} = \sum_i m_i(x_i^2 + z_i^2) = 2m_H(0.7578 \times 10^{-8})^2$$

and

$$I_{xy} = 0$$

$$I_{xz} = m_H(0.50588) * 0.7578 + m_H(0.50588) * (-0.7578) = 0$$

$$I_{yz} = 0$$

where

$$m_H \sim \frac{1}{6 \times 10^{23}} = 1.66666 \times 10^{-24} grams$$

and

$$m_O \sim \frac{16}{6 \times 10^{23}} = 2.6666 \times 10^{-23} grams$$

.

$$I_{yy} = 2 \times 1.666 \times 10^{-24} \times (0.7578 \times 10^{-8})^2 = 1.91 \times 10^{-40} gram\ cm^2$$

$$I_{xx} = \frac{16}{6 \times 10^{23}}(0.0652 \times 10^{-8})^2 + 2\frac{1}{6 \times 10^{23}}(0.5425 \times 10^{-8})^2 = 1.09 \times 10^{-40} gram\ cm^2$$

The tensor of the moment of inertia is now given by

$$\begin{pmatrix} 1.09 \times 10^{-40} & 0 & 0 \\ 0 & 1.91 \times 10^{-40} & 0 \\ 0 & 0 & 3.00 \times 10^{-40} \end{pmatrix}$$

and it is conventional to define the "major" axis as "A",

the "minor" axis as "C", and the intermediate one as "B". The ordering is the $I_A < I_B < I_C$. An "oblate symmetric top" is one for which $I_A = I_B < I_C$, whereas a "prolate symmetric top" has $I_A < I_B = I_C$.

IV. THE ENERGY LEVELS FOR AN PROLATE SYMMETRIC TOP

The Hamiltonian is

$$H_{op} = \frac{L_A^2}{2I_A} + \frac{L_B^2}{2I_B} + \frac{L_C^2}{2I_C}$$

which we re-write as

$$H_{op} = \frac{L_A^2}{2I_A} + \frac{1}{2I_B}\left(L_B^2 + L_C^2\right)$$

or

$$H_{op} = \frac{L_A^2}{2I_A} + \frac{1}{2I_B}\left(L^2 - L_A^2\right)$$

which re-arranges to

$$H_{op} = \frac{L_A^2}{2I_A} - \frac{1}{2I_b}L_A^2 + \frac{1}{2I_B}L^2$$

so, if L_A is associated with L_z one has

$$E_{J,K} = \left(\frac{1}{2I_A} - \frac{1}{2I_B}\right)K^2\hbar^2 + \frac{1}{2I_B}J(J+1)\hbar^2$$

J is the familiar total rotational angular momentum quantum number, while K is related to the projection of J on the molecular symmetry axis. The normal selection rules for this kind of molecule turn out to be $\Delta J = \pm 1$ (no surprise there), and $\Delta K = 0$.

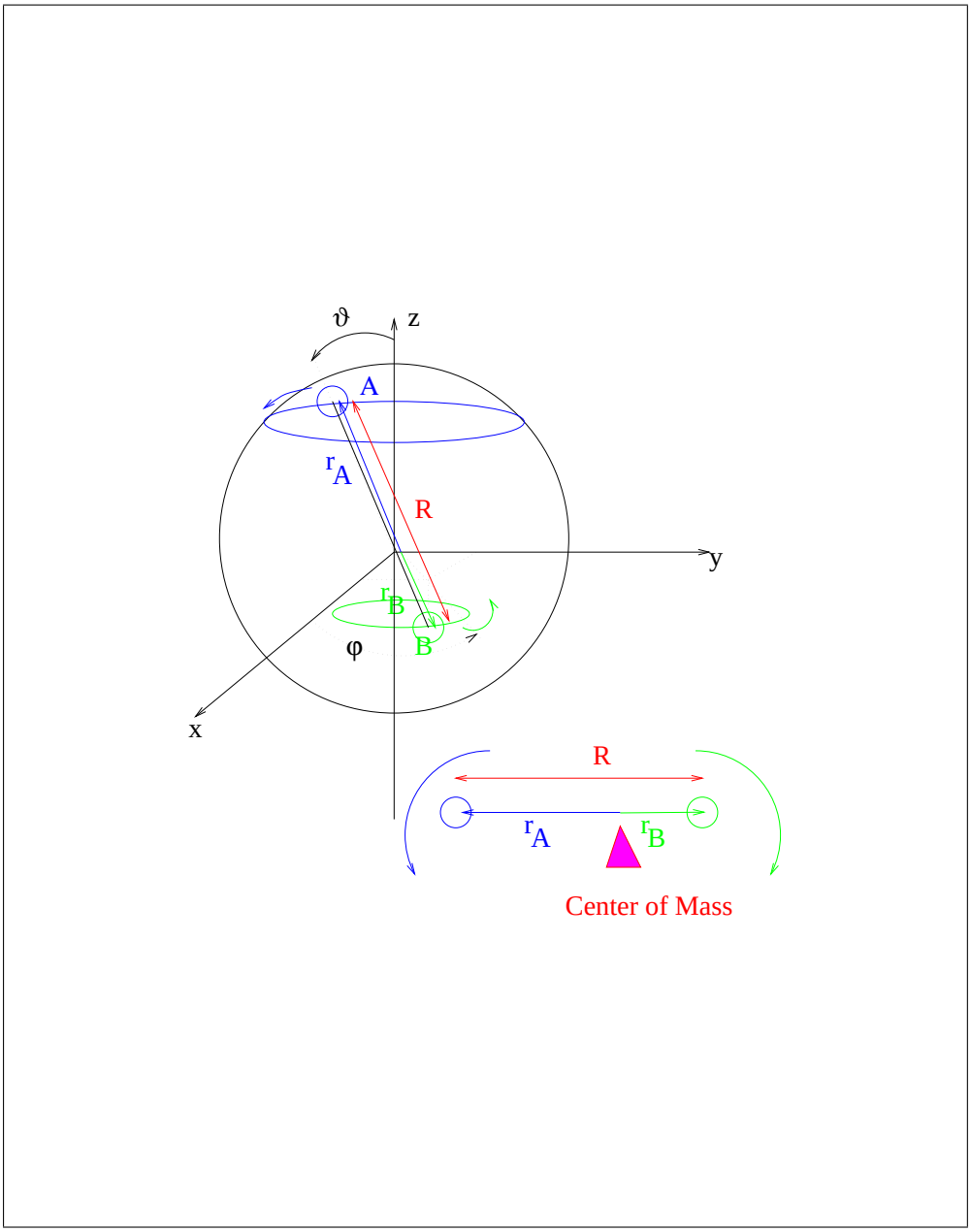

FIG. 1: The diatomic A-B molecule, in the center of mass coordinate system.

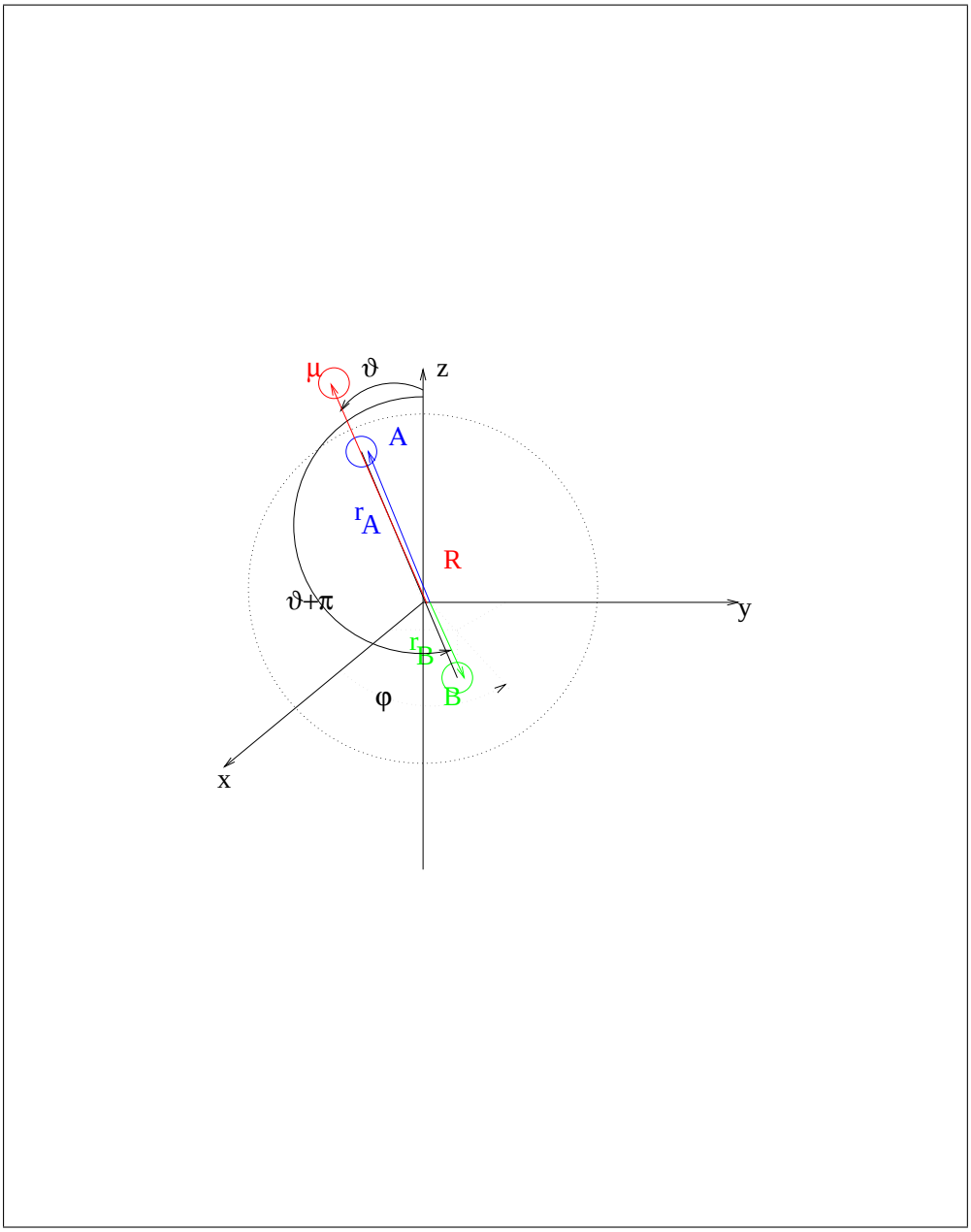

FIG. 2: The diatomic A-B molecule, in the center of mass coordinate system. The pseudo particle, μ), is shown in red.

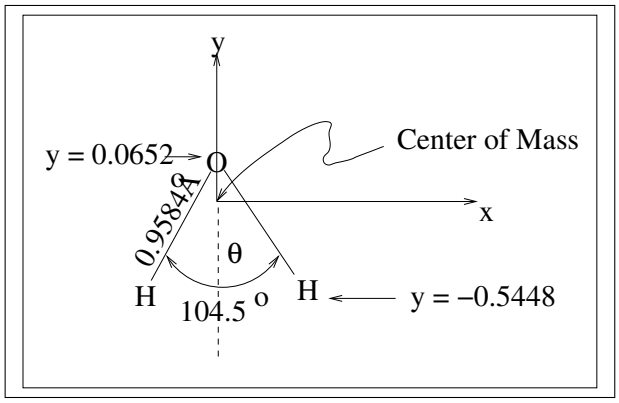

FIG. 3: Water, in the x-y plane