Appendix A

Moment of inertia for a linear triatomic molecule

The inertia tensor \( \mathbf{I} \) is a second-rank Cartesian tensor \([142]\),

\[
\mathbf{I} = \begin{pmatrix}
I_{xx} & I_{xy} & I_{xz} \\
I_{yx} & I_{yy} & I_{yz} \\
I_{zx} & I_{zy} & I_{zz}
\end{pmatrix}.
\] (A.1)

The diagonal elements \( I_{jj} \) are called the \textit{moments of inertia}, and the off-diagonal elements \( I_{jk} \) are referred to as the \textit{products of inertia}. A particular set of Cartesian coordinates \( x, y, \) and \( z \) can be chosen such that the axes pass through the center of mass of the body and the \textit{products of inertia} vanish \([162]\). The moments of inertia about the principle \( x, y, \) and \( z \) axes are the \textit{principle moments of inertia}, \( I_{xx}, I_{yy}, \) and \( I_{zz} \), respectively, and are given as:

\[
I_{xx} = \sum_{i=1}^{n} m_i \left[ (y_i - y_{c.o.m.})^2 + (z_i - z_{c.o.m.})^2 \right] \quad \text{(A.2)}
\]

\[
I_{yy} = \sum_{i=1}^{n} m_i \left[ (x_i - x_{c.o.m.})^2 + (z_i - z_{c.o.m.})^2 \right] \quad \text{(A.3)}
\]

\[
I_{zz} = \sum_{i=1}^{n} m_i \left[ (x_i - x_{c.o.m.})^2 + (y_i - y_{c.o.m.})^2 \right] \quad \text{(A.4)}
\]

where \( n \) is the number of atoms and \( e.g. x_i - x_{c.o.m.} \) is the \( x \) component of the vector \( \vec{r}_i \) to the \( i \)th mass from the center of mass. The total mass of the system, \( M \), is given as the sum over \( n \) masses,

\[
M = \sum_{i=1}^{n} m_i. \quad \text{(A.5)}
\]
The three principle moments of inertia are labelled $I_{aa}$, $I_{bb}$, and $I_{cc}$, where by convention, $I_{cc}$ is the largest and $I_{aa}$ is smallest [142]:

$$I_{cc} \geq I_{bb} \geq I_{aa} \quad (A.6)$$

Next, we consider the specific case of a triatomic linear molecule, ABC, whose masses $m_A$, $m_B$, and $m_C$ lie along the molecular axis that rotates about a space-fixed $Z$ axis through the molecule’s center of mass, labelled $Z_{c.o.m.}$ (see Figure A.1). Since the masses of the nuclei lie on the $a$ axis, the distance from the $i$th mass to the $a$ axis is zero, and

$$I_{cc} = I_{bb} > I_{aa} = 0. \quad (A.7)$$

The moment of inertia about the axis through the center of mass is then

$$I_{Z_{c.o.m.}} = m_A R_A^2 + m_B R_B^2 + m_C R_C^2. \quad (A.8)$$

Here, $R_A$, etc. are distances from the masses to the center of mass. With help of the Parallel Axes Thereom, a transformation can be made to recast Eq. (A.8) in terms of its bond lengths [144]:

**Parallel Axes Thereom**: Let the c.o.m. be the center of mass of a rigid body. Let $Z_{c.o.m.}$ be an axis through the c.o.m.. Let $Z$ be another axis parallel to $Z_{c.o.m.}$. Then

$$I_Z = I_{Z_{c.o.m.}} + M d^2 \quad (A.9)$$

where $M$ is the mass of the body and $d$ is the perpendicular distance between the two axes.

Applying the Parallel Axes Thereom, one obtains

$$I_{Z_{c.o.m.}} = \frac{m_A R_{AB}^2 + m_C R_{BC}^2}{I_Z} - M d^2 \quad (A.10)$$
where
\[ d = \left( \frac{m_A R_{AB} - m_C R_{BC}}{M} \right) \]  \hspace{1cm} (A.11)

and
\[ M = m_A + m_B + m_C. \]  \hspace{1cm} (A.12)

Simplifying Eq. (A.10), one obtains,
\[ I_{Z.c.o.m.} = m_A R_{AB}^2 + m_C R_{BC}^2 - \frac{1}{M} (m_A R_{AB} - m_C R_{BC})^2. \]  \hspace{1cm} (A.13)
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