A Quick Look at THz Attenuation Mechanisms and Propagation

Two types of attenuation, both more common than in lower RF bands:

(1) Absorption
- Conversion of electromagnetic radiation into heat
(a) Conduction current (Joule) heating: \( P_{\text{diss}} = \overline{J \cdot E} \)
  (e.g., losses in undepleted semiconductors)
  (overbar denotes time average)
(b) Polarization current heating \( P_{\text{diss}} = (\frac{dP}{dt}) \cdot E \)
  (e.g., polar liquids, such as water in a microwave oven)

(2) Scattering
(a) Non-resonant internal scattering from inhomogeneous dielectrics
  (e.g., composite materials such as RT-Duroid)
(b) Resonant scattering from particles of dimension \( \sim \lambda \) (e.g., raindrops)
(c) Mixture of specular scattering from smooth surfaces and diffuse scattering from rough surfaces (in infrared, more surfaces tend to be diffuse; in RF bands more surfaces tend to be specular)
Radiative Transfer

\[ \frac{dB}{dr} + \alpha B = \frac{\rho J}{4\pi} \]

1D Radiative Transport Equation

\[ \alpha \rightarrow \text{attenuation constant} \quad \rho \rightarrow \text{density} \quad J \rightarrow \text{emission coefficient} \]

\[ B(r) = B_s \exp(-\tau) + (\rho J/4\pi\alpha)[1 - \exp(-\tau)] \]

\[ \tau = \int_0^L \alpha(r)dr \]

Homogeneous Solution \quad Particular Solution \quad “Optical Depth”

Special Cases: (1) \( j = 0 \Rightarrow B = B_s \exp(-\tau) \) \quad Beer-Lambert Law

(2) \( B = \text{uniform} \Rightarrow dB = 0 \Rightarrow B = (\rho J/4\pi\alpha) \) \quad Kirchoff’s Law

Describes attenuation effects for many THz point sensors (active and passive), and for remote active systems. Especially useful when intervening material is a linear, isotropic, and homogeneous (LIH) dielectric, or an array of independent scatterers:

\[ T \equiv \frac{I_t}{I_i} = \exp(-\alpha_A \cdot z) \quad T \rightarrow \text{transmission, } \alpha_A \rightarrow \text{attenuation coefficient} \]

\[ I_i \rightarrow \text{incident intensity, } I_t \rightarrow \text{transmitted intensity} \]

For absorption, \( \alpha_A = \alpha_{\text{ABS}} \), the absorption coefficient
(a characteristic of the material, and generally a function of frequency)

For scattering \( \alpha_A = \rho \sigma_S \), \( \rho \) being the density and \( \sigma_S \) the scattering cross section
Simulation Tool:
• Windows®-based atmospheric propagation tool called PcLnWin (Ontar, Corp.)
• FASCODE radiative transfer engine developed by U.S. Air Force Geophysics Lab in 1970s.
• HITRAN96 database (> 1 million molecular lines) developed by molecular chemists and maintained by U.S. Air Force (Hanscom AFB)

Atmospheric Conditions
• Seven “standard” molecules: H₂O, CO₂, O₃, N₂O, CO, CH₄, O₂

• 1976 U.S. standard atmospheric model @ sea level
  - Temperature = 288 K, Pressure = 1 atm, Humidity = 46%

Between 300 GHz and 2.0 THz, water vapor dominates the attenuation by way of molecular dipole transitions
Stick Diagram of Atmospheric Molecular Lines

Line Strength [cm$^{-1}$/(molecule-cm$^2$)]

Frequency [GHz]

100 200 300 400 500 600 700 800 900 1000

1E-30 1E-28 1E-26 1E-24 1E-22 1E-20

183.4 325.4 380.5 448.3 475.0 548.0 621.1 752.6 916.8 971.0 988.6
Why is Water Vapor Absorption So Strong and So Complicated?

• For all polar molecules in the vapor state, THz transitions can occur between angular momentum eigenstates of the entire molecule if the energy difference between eigenstates = $h\nu$, and if the change in angular momentum along the axis of photon propagation = $h/2\pi$

• For symmetric rotors (e.g., carbom monoxide CO, hydrogen chloride HCl, etc.), two of the moments (along two orthogonal axes) are identical and the third is trivially small, so that

$$I_x \rightarrow \text{moment of inertia for rotation about a given axis, } x$$

$$L \rightarrow \text{orbital angular momentum eigenvalue}$$

Photon absorption or emission can occur of $\Delta l = 1$, for which

$$\Delta U = \frac{\hbar^2}{2I_x} [(l+1)(l+2) - l(l+1)] = \frac{\hbar^2}{I} (l+1) = \hbar \omega$$

This creates a “ladder” of photon frequencies as shown to the right

• Although highly polar, water is asymmetric rotor meaning that no two moments of inertia are equal. This follows from its non-collinear alignment between the three atoms

• Any of these purely rotational transitions will be easily observed if $\omega\tau >> 1$  where $\tau$ is the momentum relaxation time (or dephasing time)

• Generally, $\tau > 100$ ps or more under STP conditions, so THz transitions are obvious
Atmospheric Simulation, Propagation “Windows”

Absorption [dB/km]

Frequency [THz]

- 260 GHz “Window”
- 650 GHz “Window”
- 860 GHz “Window”

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Equivalent Attenuation Length

* Since Lambert-Beer law of transmission, $T = \exp(-\alpha z)$ applies the $1/e$ attenuation length is a “natural” metric.
Ten Strongest Water Vapor Lines in THz Region
(the big “whoppers”)

<table>
<thead>
<tr>
<th>Freq [THz]</th>
<th>Peak Attenuation [dB/m]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.558</td>
<td>18.4</td>
</tr>
<tr>
<td>0.758</td>
<td>12.7</td>
</tr>
<tr>
<td>0.989</td>
<td>9.4</td>
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<tr>
<td>1.098</td>
<td>61.6</td>
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<tr>
<td>1.164</td>
<td>71.6</td>
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<td>1.412</td>
<td>52.9</td>
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<tr>
<td>1.671</td>
<td>163.6</td>
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<tr>
<td>1.718</td>
<td>150.0</td>
</tr>
<tr>
<td>1.869</td>
<td>59.9</td>
</tr>
<tr>
<td>1.920</td>
<td>46.3</td>
</tr>
</tbody>
</table>
Absorption Models for Liquids and Solids

(1) Drude model of conductors:

\[ \varepsilon = \varepsilon_{\text{back}} - j \frac{\sigma}{\omega} \quad \sigma = \frac{\sigma_0}{1 - j\omega\tau} \]

- \( \tau \rightarrow \) momentum relaxation time
- \( \sim 10 \text{ fs in common metals @300 K} \)
- \( > 100 \text{ fs in semiconductors @300 K} \)

(2) Debye model of polar liquids (single component):

**Single Debye**

\[ \varepsilon = \varepsilon_{\infty} + \frac{\varepsilon_0 - \varepsilon_{\infty}}{1 + j(\nu / \nu_1)} \]

**Double Debye**

\[ \varepsilon = \varepsilon_{\infty} + \frac{\varepsilon_0 - \varepsilon_1}{1 + j(\nu / \nu_1)} + \frac{\varepsilon_1 - \varepsilon_{\infty}}{1 + j(\nu / \nu_2)} \]

e.g., for pure water at 300 K, single Debye relaxation frequency \( \nu_1 = 17.5 \text{ GHz} \),
and the dielectric constants \( \varepsilon_0 \) and \( \varepsilon_{\infty} \) are 79.7 and 5.26, respectively

(3) Independent of absorption model, Maxwell’s eqns predict:

\[ \alpha = 2\omega \left\{ \frac{\mu \varepsilon'}{2} \left[ \sqrt{1 + (\varepsilon'' / \varepsilon')^2} - 1 \right] \right\}^{1/2} \]

where \( \varepsilon \equiv \varepsilon' + j\varepsilon'' \)
Single-Debye Model for Liquid Water

\[(\varepsilon_0 = 78.2, \varepsilon_\infty = 4.9, \tau = 8.1 \text{ ps, all at } 25^\circ C)\]
(\(\varepsilon_0 = 78.2, \varepsilon_\infty = 4.9, \tau = 8.1 \text{ ps}, \text{ all at } 25^\circ\text{C}\))
Scattering from a Conducting Sphere

First Mie resonance

Rayleigh limit, $\sigma \to (a/\lambda)^4$

[O. V. Blake, "Radar Range Performance Analysis," (Artech House, Norwood, MA, 1986), Fig. 3-1].
The maximum is $\sigma \approx 3.65 \pi a^2$ at $a = 0.163 \lambda$. This is called resonant (Mie) scattering and is caused by constructive interference of surface currents flowing around the sphere. Same effect occurs in ellipsoids and arbitrary-shaped solids… just not as strong as in spheres.

![Image of sphere and ellipsoid with surface currents](image)

Intuitive estimate of surface resonance assuming surface current velocity of $c$:

$$2\pi = \omega t = \omega (2\pi a/c) \Rightarrow a = \lambda/2\pi = 0.159 \lambda$$

Example: at 1.0 THz ($\lambda = 333 \mu m$), resonant Mie scattering occurs for a particle diameter of 106 $\mu m$.

- Many materials (e.g., powders such as sugar; composites such as RT-Duroid) have inhomogeneity on the 100 micron scale $\Rightarrow$ strong THz scattering.
UCSB Measurements

Double Debye: $\varepsilon = \varepsilon_\infty + \frac{\varepsilon_0 - \varepsilon_1}{1 + j\frac{\nu}{\nu_1}} + \frac{\varepsilon_1 - \varepsilon_\infty}{1 + j\frac{\nu}{\nu_2}}$

$\nu_1 = 17.4$ GHz, $\nu_2 = 693.1$ GHz, $\varepsilon_0 = 79.7$, $\varepsilon_1 = 5.35$, $\varepsilon_\infty = 3.37$ (1)

Disagreement about Salt Water

Erroneous results from the literature (NaCl-water)

Other Liquids of Varying Polarity

- Isopropyl Alcohol (5.8)
- Methanol (4.5)
- Glycerin (36)
- Water (4.6)
Common Clothing Samples

- Nylon
- Silk
- Wool
- Linen
- Denim
- Rayon
Transmission through Common Clothing

(The “Linen Closet”)

THz Transmission through Organic and Biomaterials

(The “Kitchen Cupboard”)

- Sucrose
- Powdered Calcium Sulfate (Gypsum)
- Potato Starch
- Dry
- Water Bearing
- Sodium Bicarbonate
- Corn Starch
- Wheat Flour

All Starches Type B

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C4 Explosive (~90% RDX)

Three Repeated Scans

Transmitted Signal vs. Frequency [THz]
Narrow Macromolecular Resonances (Lactose Monohydrate)

(a) Water Line

(b) Gaussian, Lorentzian, FWHM = 23 GHz, Water Line

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THz Vibrational Resonance of Lactose Monohydrate

Low-lying Sub-THz resonances can be explained only by combination of intramolecular “twisting” (hindered rotation) plus intermolecular coupling

Molecular Absorption Examples (cont)

• Recall the change in energy of a rigid diatomic rotor from the state with orbital angular momentum quantum number \( l \) to state with \( l + 1 \), consistent with absorption of a photon of energy \( h \nu \):

\[
\Delta U = \frac{\hbar^2}{2I}[(l+1)(l+2) - l(l+1)] = \frac{\hbar^2}{I} (l+1) = \hbar \omega \quad \text{or} \quad \nu = \frac{\hbar}{2\pi I} (l+1) \equiv 2B(l+1)
\]

where \( B \) is called the rotational constant and \( I \) is the moment of inertia. Recall from mechanics that the moment-of-inertia concept of any three-dimensional solid body of mass \( M \) allows us to divide the kinetic energy of the body into two terms: (1) linear KE of the center-of-mass, \((1/2)Mv^2\), and (2) angular kinetic energy of rotation about the center-of-mass point, \((1/2) I \omega^2 = L^2/(2I)\). It also allows us write

\[
\vec{L} = I \vec{\omega}
\]

Where \( \omega \) is a column vector denoting the circular frequency components for an arbitrary rotation about the \( x \), \( y \), and \( z \) axes respectively. This definition reminds us that \( I \) is actually a 3x3 matrix, called a tensor. When the rigid body can be approximated as a collection of \( N \) masses (very good approximation for any rigid molecule), and in a cartesian coordinate system

\[
I = \begin{pmatrix}
\sum_{i=1}^{N} m_i(y_i^2 + z_i^2) & -\sum_{i=1}^{N} m_i(x_i y_i) & -\sum_{i=1}^{N} m_i(x_i z_i) \\
-\sum_{i=1}^{N} m_i(x_i y_i) & \sum_{i=1}^{N} m_i(x_i^2 + z_i^2) & -\sum_{i=1}^{N} m_i(y_i z_i) \\
-\sum_{i=1}^{N} m_i(x_i z_i) & -\sum_{i=1}^{N} m_i(y_i z_i) & \sum_{i=1}^{N} m_i(x_i^2 + y_i^2)
\end{pmatrix}
\]

Note: this is a real symmetric matrix so from linear algebra can always be diagonalized!
The diagonal form is defined generically as

\[
I = \begin{pmatrix}
I_X & 0 & 0 \\
0 & I_Y & 0 \\
0 & 0 & I_Z \\
\end{pmatrix}
\]

satisfying

\[
\frac{x^2}{I_X} + \frac{y^2}{I_Y} + \frac{z^2}{I_Z} = 1
\]

where \(I_X\), \(I_Y\), and \(I_Z\) are called the “principal” moments of inertia. The right equation is that of an ellipsoid of revolution centered at \(x=0\), \(y=0\), \(z=0\), which is a convenient geometric construct to understand the principal moments. As in other tensorial quantities in physics, the relative values of \(I_X\), \(I_Y\), and \(I_Z\), reflect the inherent spatial symmetry, so the corresponding objects are given special names

1. \(I_X = I_Y = I_Z\) \(\Rightarrow\) spherical “top”
2. \(I_X = I_Y \neq I_Z\) \(\Rightarrow\) symmetric “top” (Recall definition of “top”: a solid object that can spin freely in any of three dimensions)
3. \(I_X \neq I_Y \neq I_Z\) \(\Rightarrow\) asymmetric “top”
4. \(I_X = I_Y\), \(I_Z \approx 0\) \(\Rightarrow\) “rotor”

Rules to determine the principal axes and moments:
1. Any axes of symmetry will generally be a principal axis.
   - Axis of symmetry means that when rotated about this axis, the molecule reproduces itself every \(2\pi/n\) degrees, where \(n > 2\)
2. If a molecule has an axis of symmetry with \(3 \leq n\), it will always be a symmetric “top”
Clearly “rotors” are the simplest since they are effectively one-dimensional

(1) Diatomic rotors

\[ I_X = I_Y = \frac{m_1 m_2 R^2}{m_1 + m_2} \rightarrow \mu R^2 \]

if \( m_1 = m_2 \), where \( \mu \) is the “reduced mass”

(2) Polyatomic (N) rotor

\[ I_X = I_Y = \frac{1}{2} \cdot \frac{\sum_{i=1}^{N} \sum_{j=1}^{N} m_i m_j R_{ij}^2}{\sum_{i=1}^{N} m_i} \]

(3) Example: Carbon Monoxide:  \( m_C = 12.0 \times 1.67 \times 10^{-27} \text{ KG} \), \( m_O = 16.0 \times 1.67 \times 10^{-27} \text{ KG} \), R 1.128 Ang, so that

\[ I = 1.457 \times 10^{-46} \text{ KG-m}^2 \text{, and } \frac{\hbar^2}{I} = 7.63 \times 10^{-23} \text{ J} = 0.476 \text{ meV or } \nu = 115 \text{ GHz} \]

Rotational transition “ladder”: \( \nu_0 = 115 \text{ GHz} \), \( \nu_1 = 230 \text{ GHz} \), \( \nu_2 = 345 \text{ GHz} \), etc.
For symmetric rotors (e.g., carbon monoxide CO, hydrogen chloride HCl, etc.), two of the moments (along two orthogonal axes) are identical and the third is trivially small, so that

\[ I = \mu R^2 \]

Ignoring spin, \( U_x = \frac{L^2}{2I_x} \)

\[ L^2 = \hbar^2 l(l+1) \]

- \( I_x \rightarrow \) moment of inertia for rotation about a given axis, \( x \)
- \( \hbar \rightarrow \) orbital angular momentum eigenvalue

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- Generally, \( \tau > 100 \text{ ps} \) or more under STP conditions, so THz transitions are obvious