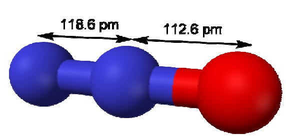
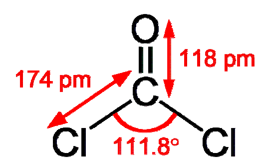
ECE594I, Prof. Brown, Fall Quarter 2009

Homework #2 Solutions: THz Propagation Phenomenology

1. Vapor State: Molecular Rotational Transitions. .
   (a) A quick Wikipedia search shows that N_2O is the linear molecule (i.e., "rotor") with bond lengths shown below. The moment of inertia is then given by
   $I = \frac{m_1 m_2 d_{12}^2 + m_1 m_3 d_{13}^2 + m_2 m_3 d_{23}^2}{m_1 + m_2 + m_3}$ where m_1, m_2 and m_3 are the masses of atoms 1, 2, and 3, respectively and can be designated arbitrarily provided d_{ij} is the corresponding distance between atom i and atom j. For the two nitrogen atoms m ~ 14 m_p and for the oxygen m = 16 m_p, where m_p is the proton rest mass. For the ground state rotational transition, we find is $\Delta U = h\nu = (\hbar^2 / I)$ or ν = 25.2 GHz, and any harmonic of this is also an allowed rotational transition So between 100 GHz and 1.0 THz, the lowest frequency transition will be the 4^{th} harmonic (at 100.7 GHz) and the highest will be the 39^{th} harmonic (at 981.5 GHz), for a total of 36 rotational transitions.
   (b) Although greatly simplified by being planar, phosgene is more complicated than a simple rotor since we need to calculate all the interatomic distances. Designating m_1 as the central carbon, m_2 as the oxygen, and m_3 and m_4 as the chlorines, we have by inspection d_{12} = 1.18 A, d_{13} = 1.74 A, d_{14} = 1.74 A. By trigonometry (law of cosines) we have for d_{23} (oxygen-chlorine distance): $(d_{23})^2 = (d_{12})^2 + (d_{13})^2 - 2\, d_{12}\, d_{13} \cos\alpha$, where α is the included angle = (360 – 111.8)/2 = 124.1°. For d_{34} (chlorine-chlorine distance) we have: $(d_{34})^2 = (d_{13})^2 + (d_{14})^2 - 2\, d_{13}\, d_{14} \cos\beta$ where β = 111.8°. These yield d_{23} = 2.59 A and d_{34} = 2.88 A. We then substitute into the following expression noting there are six unique pair-wise terms for four atoms:
   $I = \frac{m_1 m_2 d_{12}^2 + m_1 m_3 d_{13}^2 + m_1 m_4 d_{14}^2 + m_2 m_3 d_{23}^2 + m_2 m_4 d_{24}^2 + m_3 m_4 d_{34}^2}{m_1 + m_2 + m_3 + m_4}$ $=3.53\times10^{-45}$ [MKS]
   So that the ground state rotational frequency (about the axis perpendicular to the plane) is $\Delta U = h\nu = (\hbar^2 / I)$ = 4.76 GHz. This is in the microwave "C band", and is so low in frequency because chlorine is relatively heavy.





2. Liquid State: Debye Model.
   (a) Given the relaxation frequency ν_r =17.5 GHz in the course notes, $\tau = 1/(2\pi\nu_r)$ = 9.0 ps .
   We use the "single Debye model $\varepsilon = \varepsilon_\infty + \frac{\varepsilon_0 - \varepsilon_\infty}{1 + j\nu/\nu_r}$ with ε_0 = 79.7 and ε_0 =5.26 and through the use of an Excel spreadsheet, we get the following real and imaginary values of the dielectric constant, normalized to ε_0 – the permittivity of vacuum.

Freq [GHz]	Real eps	Imag eps
10	61.62	-31.93
100	7.51	-12.74
300	5.52	-4.36
1000	5.28	-1.31
3000	5.26	-0.44

Freq [GHz]	Real r	Imag r	Real t	Imag t
10	0.790	-0.046	1.790	-0.046
100	0.614	-0.170	1.614	-0.170
300	0.463	-0.134	1.463	-0.134
1000	0.401	-0.051	1.401	-0.051
3000	0.394	-0.018	1.394	-0.018

(b) From electromagnetics, the field reflection coefficient at the air-water interface is r = $(n_1-n_2)/(n_1+n_2)$, where n_1 is for the air (≈1.0) and n_2 is for the water and always given by n = $(\varepsilon)^{1/2}$
The field transmission is t =1+r = $2n_1/(n_1+n_1)$, n again being complex.
(c) Again from electromagnetics, the power reflection coefficient R = $|r|^2$ and T = $|t|^2$ = 1-R

Freq [GHz]	R	T	α [1/cm]	L [cm]	Emiss
10	0.626	0.374	8	0.1210	0.374
100	0.406	0.594	80	0.0125	0.594
300	0.232	0.768	110	0.0091	0.768
1000	0.164	0.836	119	0.0084	0.836

(d) Knowing the complex dielectric function, we can calculate the absorption coefficient at any frequency by: $\alpha = 2\omega\left\{\frac{\mu\varepsilon'}{2}\left[\sqrt{1+(\varepsilon''/\varepsilon')^2}-1\right]\right\}^{1/2}$ (found in any good book on electromagnetic fields and waves, such as F. Ulaby, "Applied Electromagnetics")

where ε = ε' + jε'' and μ is the magnetic permeability, assumed to equal $\mu_0 = 4\pi\cdot10^{-7}$ (water is generally very weakly magnetic). The attenuation length (or penetration depth) L is just 1/α, and by Kirchoff's law the emissivity = 1 – R = T.

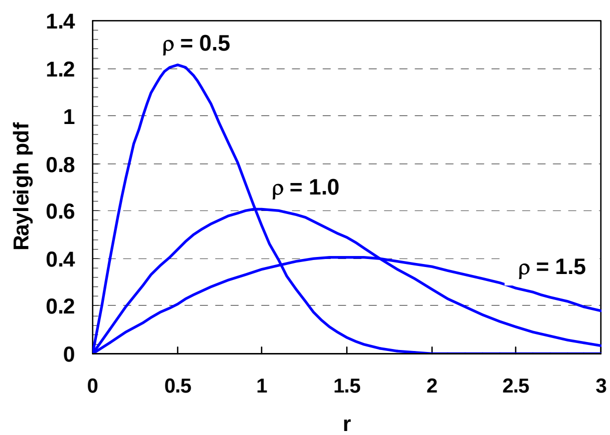
3. Solid State: Drude model.
(a) According to the Drude model, the complex conductivity is given by $\sigma = \sigma_0/(1-j\omega\tau)$
For ν = 300 GHz, τ = 0.3 ps, and three values of resistivity, 0.1, 1, and 10 Ω-cm, we get the conductivity results shown in the table in MKSA units (S/m).
(b) As for any conductor, the complex dielectric function is defined simply by $\varepsilon = \varepsilon_b - j\sigma/\omega$ where ε_b is the "background" dielectric constant. These values are easy to compute from the complex σ values and included in the table below. Note that they are given as relative values $\varepsilon/\varepsilon_0$, where ε_0 is the permittivity of vacuum.
(c) To get the absorption coefficient [cm^{-1}] and penetration depth we use the same formula as for the water in Problem 2(d). The results are included in the table. Notice that even for the 10 Ω-cm silicon, the absorption coefficient at 300 GHz is ~8.15 cm^{-1}, or equivalently the penetration depth is only 1.2 mm, which are prohibitively lossy for integrated circuit applications. This is why people who develop silicon ICs at mm-wave and THz frequencies generally use "high resistivity" substrates having ρ > 10^4 Ω-cm. Note that GaAs and InP can both be prepared in substrates having much higher resistivity, so called "semi-insulating" substrates having ρ > 10^6 Ω-cm.

	Sample 1	Sample 2	Sample 3
dc resistivity [Ohm cm]	0.1	1	10
dc conductivity [S/m]	1000	100	10
tau [s]	3E-13	3E-13	3E-13
epsilon zero	12	12	12
Frequency [GHz]	300	300	300
Real conductivity [S/m]	757.70	75.77	7.58
Imag conductivity [S/m]	428.47	42.85	4.28
Real epsilon	37.68	14.57	12.26
Imag epsilon	-45.42	-4.54	-0.45
Abs Coeff (1/cm)	410.61	73.93	8.15
Penetration depth [cm]	0.0024	0.0135	0.1226

4. Scattering Effects: THz propagation through fog (plus good exercise in probability)

It is well known that microwaves and millimeter waves have far better transmission through clouds and fog than infrared or visible light. But what about THz transmission ? Provided that the water particles in the fog are all spherical and much smaller than a wavelength so that the scattering is in the Rayleigh limit, the radar cross section of an individual water droplet can estimated by the expression derived from effective-medium theory of optics: $\frac{\sigma}{\pi R^2} = 4\left|\frac{\varepsilon_c - 1}{\varepsilon_c + 2}\right|^2 \left(\frac{2\pi R}{\lambda}\right)^4$ where R is the radius and ε_c is the complex dielectric function.

Assume the distribution function of droplets can be approximated as a Rayleigh pdf with the most likely radius being 10 micron and the concentration of fog particles being 50 cm^{-3}.



(a) The Rayleigh probability density function is very useful in sensor analysis of all types, including THz systems. It is the "single-sided" function given by

$p(r) = \frac{r}{\rho^2}\exp(-r^2/2\rho^2)$ with r ranging from 0 to infinity. The behavior of the Rayleigh pdf for three different values of the variance is seen below. Note that the most likely value (i.e., where the pdf reaches its maximum) of r is equal to ρ. This can be confirmed by setting the 1st derivative to zero: $\frac{dp}{dr} = \frac{\exp(-r^2/2\rho^2)}{\rho^2}\left(\frac{-2r^2}{2\rho^2}+1\right) = 0 \Rightarrow r = \rho$. Hence, ρ = 10 micron and the variance $\rho^2 = (100\ \mu m^2)$.

(b) To get the mean value of the cross section, we consider the radius as a random variable and use the formula given to write: $\sigma = \frac{64\pi^5}{\lambda^4}\left|\frac{\varepsilon_c - 1}{\varepsilon_c + 2}\right|^2 r^6$. By probability theory, the mean value is simply $<\sigma>= \frac{64\pi^5}{\lambda^4}\left|\frac{\varepsilon_c - 1}{\varepsilon_c + 2}\right|^2 \int_0^\infty \frac{r^7}{\rho^2}\exp(-r^2/2\rho^2)dr$, which is an analytic "Gaussian" integral. Use of an old-fashioned integral table (or a symbolic computer tool such as Maple or Mathematica) yields the very useful formula $\int_0^\infty x^{2n+1}\exp(-ax^2)dx = \frac{n!}{2a^{n+1}}$, so setting n = 3 and equating a to $(2\sigma^2)^{-1}$, we get $<\sigma>= \frac{64\pi^5}{\lambda^4}\left|\frac{\varepsilon_c - 1}{\varepsilon_c + 2}\right|^2 \frac{6}{\rho^2}\frac{(2\rho^2)^4}{2} = \frac{3072\pi^5}{\lambda^4}\left|\frac{\varepsilon_c - 1}{\varepsilon_c + 2}\right|^2 \rho^6$

We now use the spreadsheet (or MATLAB script) developed in Problem 2 above to get the magnitude $|(\varepsilon_c - 1)/(\varepsilon_c + 2)|$, and then the mean value of the radar cross section at 10 GHz, 100 GHz, 300 GHz, and 1.0 THz using the "single-Debye" model for the dielectric function of water. The results are given in the table below.

(c) For individual single-particle scattering, $\alpha \approx N_d <\sigma>$ where N_d is the concentration of droplets ($5.0\text{x}10^5/\text{m}^3$). The value for α is listed in the table below at 10, 100, 300, and 1000 GHz. The attenuation in dB/km is found by taking the logarithm of Beer's exponential decay function, $-10*\log_{10}[\exp(-\alpha * 1000)]$ where here a is in units m^{-1}. Note from the table that the fog remains highly transparent until 1000 GHz. Please note, however, that this calculation ignores the effect of the water vapor that always comes with fog. The droplets are just a result of nucleation that occurs when the air becomes saturated with water vapor. The water vapor absorption will likely dominate the fog attenuation in all practical scenarios. However, it is interesting to see what contribution the fog particles make.

Freq [GHz]	Mean RCS [m^2]	Atten Coeff [1/cm]	dB/km
10	1.08E-18	5.38E-13	2.33E-07
100	9.40E-15	4.70E-09	2.04E-03
300	4.91E-13	2.45E-07	1.07E-01
1000	4.25E-11	2.13E-05	9.24E+00

Also note that the most likely fog particle RCS is $\pi(10\ \mu\text{m})^2 = 3.1\text{x}10^{-10}\ \text{m}^2$. Since the mean RCS is much less than the geometric limit even at 1.0 THz, we have some faith that the fog particles are still in the Rayleigh limit at this frequency.