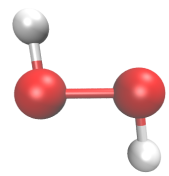
CHEM 1000 Fall 2016
Practice Exam 1 Name: ______________________________

Show your work to receive full credit. You have 60 minutes to take this 100 point exam. (Note: The real exam will be a little shorter and require 45 minutes.)

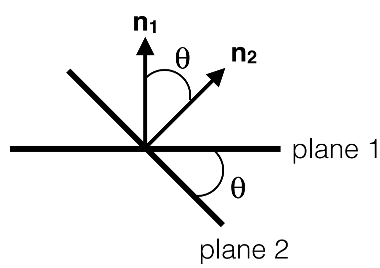
1. (*30 points*) Below are the XYZ coordinates for a hydrogen peroxide molecule:

O1	-2.320	0.697	2.202
H1	-2.440	1.572	2.617
O2	-0.866	0.709	2.207
H2	-0.746	-0.167	1.792



(a) Calculate the O1-H1 distance. (10 P)

(b) The atoms O1-H1-O2 and O2-H2-O1 define two planes. What is the angle between these two planes? The sketch below may help you. (20 P)



2. (*34 points*) Determine the solutions to the following equations:

(a) $x^5 = 243$. Solve exactly and sketch your solutions in Cartesian form. (8 Pts)

(b) $2x^2 + 3x - \sin(x) = 1$. Solve using linearization. (8 Pts)

(c) $x^3 + 2x^2 - x + \alpha = 0$. Solve approximately by assuming that α is very small. (8 Pts)

(c) $x^3 + 2x^2 - x + \alpha = 0$ with $\alpha = \frac{1}{10}$. Solve approximately using the iterative approach. Use only two iterations to keep the work manageable. (10 Pts)

3. (*36 points*) Multiplying a vector by the matrix

$$\mathbf{D} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$$

corresponds to rotating the vector by an angle θ.

(a) Is this matrix (1) Hermitian, (2) orthogonal, or (3) unitary? (6 Pts)

(b) Calculate the vector resulting from rotating $\vec{x} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ by $\theta = \frac{\pi}{4}$. (10 Pts)

(c) Determine the eigenvalues λ and eigenvectors $\vec{x}$ of $\mathbf{D}$. (10 Pts)
Hint: You should obtain $\lambda_{1,2} = e^{\pm i\theta}$, $\vec{x}_1 = N \cdot \begin{pmatrix} 1 \\ -i \end{pmatrix}$ and $\vec{x}_2 = N \cdot \begin{pmatrix} -i \\ 1 \end{pmatrix}$, where N is a normalization constant. You do not need to determine N.

(d) Calculate the matrix inverse $\mathbf{D}^{-1}$, i.e. the matrix undoing rotation by θ. Check your result by calculating $\mathbf{D}^{-1} \cdot \mathbf{D}$. (10 Pts)
Hint: There is a simple, intuitive solution that allows you to skip the cumbersome calculation of the inverse.

4. (*20 points*) BONUS:

(a) Show that Hermitian matrices have real eigenvalues. (10 Pts)

(b) Show that Hermitian matrices have orthogonal eigenvectors. (10 Pts)