NAME/TEAM: _____

Summer Teaching Program in Environmental Chemistry
Computational Chemistry Laboratory Worksheet

Using Spartan to Investigate the Molecular Properties of Atmospherically Relevant Greenhouse Gases
Last modified: June 17, 2014

1. Geometry optimization

(a) Perform the optimization of the geometry of each molecule as described in the lab manual and enter the calculated values of the geometric parameters in the table below.

molecule	parameter	values	
		calculated	experimental (CRC)
CO_2	CO bond (Å)		
	OCO angle (°)		
H_2O	OH bond (Å)		
	HOH angle (°)		
N_2O	NN bond (Å)		
	NO bond (Å)		
	NNO angle (°)		
O_3	OO bond (Å)		
	OOO angle (°)		

(b) Look up experimental values of the geometric parameters in the online CRC Handbook (www.hbcponline.com) and add them to the table.

(c) Briefly discuss the level of agreement between your calculated geometric parameters and the corresponding experimental values.

2. Vibrational analysis

(a) Perform the computation of the vibrational frequencies of each molecule as described in the lab manual and enter the values in the following table:

molecule	mode	frequencies (cm^{-1})		IR active?	experimental wavelength (μm)	overlap with BB spectrum?
		calculated	experimental (NIST)			
CO_2	sym. str.					
	asym. str.					
	bend					
H_2O	sym. str.					
	asym. str.					
	bend					
N_2O	NN str.					
	NO str.					
	bend					
O_3	sym str.					
	asym. str.					
	bend					

(b) Look up experimental values of the vibrational frequencies in the NIST database (http://webbook.nist.gov/chemistry/form-ser.html) and add them to the table.

(c) Briefly discuss the level of agreement between your calculated vibrational frequencies and the corresponding experimental values.

3. Charge distribution

Examine the electrostatic potential surface of each molecule to get an idea of how the charge is distributed. In the space below, sketch the molecules and label each atom with partial charges (i.e., δ^+ or δ^-). Draw arrows indicating the direction of the bond dipoles. Indicate whether or not the molecule has a net dipole moment.

(a) CO_2 (b) H_2O

(c) NO_2 (d) O_3

4. Infrared activity

Animate each of the vibrational modes of your molecule. In the space below, make a sketch of each vibrational mode, using double-headed arrows the relative motion of the atoms for each mode. Indicate which modes are IR active (i.e., change the dipole moment of the molecule) in the vibrational analysis table on p. 2.

(a) CO_2

(b) H_2O

(c) N_2O

(d) O_3

5. Overlap of IR active modes with Earth's blackbody radiation spectrum

(a) For each IR active mode of each molecule, convert the experimental vibrational frequency in cm^{-1} to wavelengths in μm, and enter the result in the vibrational analysis table on p. 2.

(b) Compare the wavelengths of the IR active modes with Earth's theoretical blackbody radiation spectrum (found on the last page of the COMPUTATIONAL CHEMISTRY LAB MANUAL). Indicate in the vibrational analysis table on p. 2 which modes absorb radiation at wavelengths that overlap with the theoretical blackbody (BB) spectrum. Do you see evidence of absorption from the modes you identified in the experimentally measured spectrum of radiation leaving the upper atmosphere?