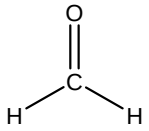
6 Modeling in Solution

Exercise 1 Will a Molecule of Water Pass through the Center of a Molecule of Benzene?

Build a molecule of H_2O and optimize using PM3.
Save as h2opm3.HIN.
Open and new worksheet and build a molecule of C_6H_6. Optimize using PM3.
Save as c6h6pm3.HIN.
Click File / Merge and select h2opm3.HIN.
Does it look like there is an empty space in the center of the benzene molecule through which the water molecule can pass? _____
Click Display / Rendering: Sticks and Dots and click OK.
Is there an empty space in the center of the benzene molecule through which the water molecule can pass? _____
Close.

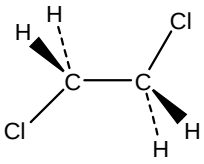
Exercise 2 Determine the Frequency Shift for C=O for Formaldehyde Dissolved in Water.

Build a molecule of CH_2O.
Minimize using PM3 and save as ch2ogas.HIN.
Determine the vibrational/IR spectrum by clicking Compute / Vibrations.

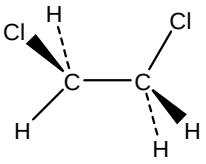


Click Compute / Vibrational Spectrum. Click the various peaks and use the animation option to observe the vibrational modes. The most intense peak is the C=O stretch. Record the value $\tilde{\nu}$ = _____ cm^{-1} (literature 1746.07 cm^{-1}).
Save.
Save as ch2osoln.HIN.
Click Setup / Periodic Box. Enter 12, 12, 12 and click OK.
Click Display / Rendering / Sticks: Perspective and click OK.
Click Compute / Vibrations. (Note that this calculation will take a few hours.) Click Compute / Vibrational Spectrum. Click some of the bands to observe the solvent vibrations and some of the various peaks to observe the formaldehyde peaks. The most intense peak is the C=O stretch. Record the value $\tilde{\nu}$ = _____ cm^{-1} (literature 1723 cm^{-1}).
The difference between these frequencies is the effect on the vibrational frequency as a result of the solvation process. $\Delta\tilde{\nu}$ = _____ cm^{-1}.
Save.

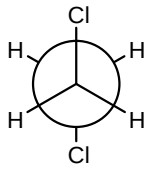
Exercise 3 Determine the Stable Form of 1,2-dichloroethane.

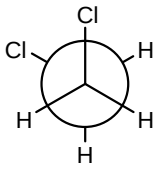


trans



gauche





Build a molecule 1,2-dichloroethane. The *trans* conformer will appear.

Minimize at the MM+ level and save as c2h4cl2gastransmm.HIN. Record the value of the energy E = _____ kcal mol^{-1}.

Change the *trans* conformer to the *gauche* conformer by defining the Cl-C-C-Cl dihedral angle and clicking Build / Constrain Torsion: Gauche. Click OK. Right click in the workspace and double click the Selection Tool.

Save as c2h4cl2gasgauchemm.HIN.

Minimize at the MM+ level and record the value of the energy E = _____ kcal mol^{-1}.

Save.

Which conformer is more stable in the gaseous phase and by how much energy?

_____ conformer by _____ kcal mol^{-1} (literature 1.1 kcal mol^{-1}).

Close.

Open c2h4Cl2gastransmm.HIN and save as c2h4Cl2solntransmm.HIN.

Click Setup / Periodic Box and enter 12, 12, 12. Click OK.

Minimize the molecule in aqueous solution using MM+.

Save and record the energy _____ kcal mol^{-1}.

Close and open c2h4cl2gasgauchemm.HIN and save as c2h4cl2solngauchemm.HIN.

Minimize the molecule in aqueous solution as above, save, and record the energy _____ kcal mol^{-1}.

Which conformer is more stable in the gaseous phase and by how much energy?

_____ conformer by _____ kcal mol^{-1} (literature 0.3 kcal mol^{-1}).

Click Display / Rendering / Sticks and be sure that Perspective in unselected.

Close.