Intermolecular forces

Bởi:

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Intermolecular forces are interactions between individual atoms or molecules. Depending the strength of these forces, the state of the matter of these molecules can be a gas, liquid, or solid. There are four types of intermolecular forces, namely dispersion, dipole-dipole, hydrogen bonding, and ion-dipole.

Dispersion: Weak interaction with the magnitude often less than 1 kcal/mol exists between all atoms and molecules.

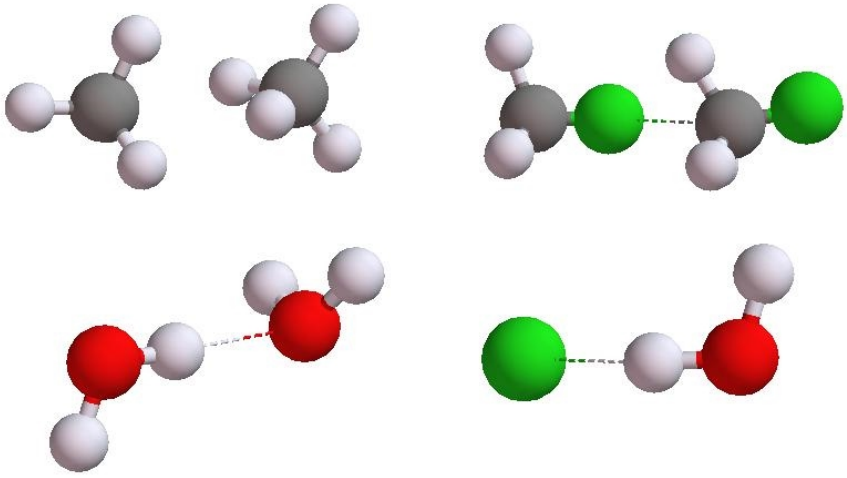
Dipole-Dipole: Slightly stronger interaction with magnitude in the range 1-3 kcal/mol exists between polar molecules.

Hydrogen bonding: A special type of dipole-dipole interaction where a hydrogen atom of one molecule directly pointing to a F, O, or N atom of the other molecule creating a rather strong dipole-dipole interaction in the range of 3-5 kcal/mol.

Ion-dipole: Strong interaction with magnitude ranging from 5-30 kcal/mol between an ion and a polar molecule.

These forces are still much weaker than a typical chemical bond, which requires about 100 kcal/mol to break.

This experiment is designed to provide an understanding on nature and the relative strength of these intermolecular forces using tools in Avisto. You can download these tools from Astonis.



Procedure:

Step 1: Use MolDesign to create monomer (isolated molecule) and a dimer for

- Methane, CH4. In the methane dimer put the distance between the two carbon atoms about 3 angstrom.
- CH3Cl. In the dimer, position the Cl atom of one molecule pointing at the methyl backend of the other with the Cl-C distance about 3 angstrom.
- Water, H2O. In the dimer, pointing the hydrogen atom on one molecule toward the oxygen of the other at a distance about 2 angstrom.
- Cl anion and Cl-....H2O complex. In the complex, pointing the hydrogen atom toward the Cl anion.

Step 2: Use Basic QChem Edu or Basic QChem to search for the stable structures of both the monomer and dimer.

Step 3: Analyze the results using PsiViewer (double click on the data sent out by step 2)

Species	Heat of formation (kcal/ mol)	Dipole (Debye)	X.....H distance (angstrom)	Binding Energy (kcal/ mol)
CH4			----------	----------
(CH4)2				
CH3Cl			----------	----------
(CH3Cl)2				
H2O			----------	----------

(H2O)2				
Cl-			----------	----------
Cl-..H2O				

1. In the fourth column record the distance between the heavy atom of one molecule to the nearest hydrogen atom of the other.
2. Calculate the binding energy = Heat of formation of the dimer - 2*Heat of formation of the monomer.

Step 4: Identify the nature of the interaction between two methane, two CH3Cl, and two water molecules.