Inorganic Chemistry with Doc M.

Day 4. Intermolecular forces.

Topics:

1. Classes of bonding within substances

covalent bonding, ionic bonding, metallic forces, network covalents

2. Intermolecular forces

dipole-dipole forces, hydrogen-bonding, instantaneous dipoles, ion-dipoles

3. Predicting physical states at room temperature

1. Classes of bonding within substances

A. Covalent bonds

C-C	ΔH = 347 kJ/mol
H-H	ΔH = 431 kJ/mol
F-F	∆H = 155 kJ/mol

B. lonic forces ($E = Z^+Z^-/r$)

LiF→Li ⁺ (g) + F⁻(g)	ΔH = 755 kJ/mol (reverse of lattice energy)
LiF→ Li(g) + F(g)	∆H = 567 kJ/mol

C. Metallic forces (metal cations in a "sea of electrons": $M(s) \rightarrow M(g)$)

Fe	∆H = 416 kJ/mol
W	∆H = 849 kJ/mol
Pb	∆H = 195 kJ/mol
Hg	$\Delta H = 61 \text{ kJ/mol} (Hg(I) \rightarrow Hg(g))$

D. Network covalent forces (endless lattice of covalent bonds)

Si $\Delta H = 450 \text{ kJ/mol} (Si(s) \rightarrow Si(g))$

2. Intermolecular forces

A. Dipole-dipole forces (3 – 4 kJ/mol)

For the polar molecule: the dipole forces is given by μ = qr where q = the equal and opposite

charges in the molecule ($\delta^+,\,\delta^-$) and r is the distance between δ^+ and $\delta^-.$

For dipole-dipole forces, $E \propto \frac{-\mu_A \mu_B}{r^3}$

Molecule	Dipole?	MM (g/mol)	bp (K)
F ₂		38	85
Cl ₂		71	
CIF		55	

B. Hydrogen bonding forces (10 - 40 kJ/mol)

a. Extra-effective dipole-dipole force that occurs when N-H, O-H and F-H bonds exist.

b. For neutral molecules, oxygen has the optimal balance between bonding groups (potentially hydrogen atoms and electron pair groups; both are required for hydrogen bonding:

Atom	B groups	E-groups	Example
Ν			NH ₃
0			H ₂ O
F			HF

c. Boiling points of Groups IV, V, VI, and VII hydrides:

Molecule	MM (g/mol)	bp (^O C)	state at 25 ^O C
CH ₄	16	-164	gas
SiH ₄	32		
GeH ₄	77		

Molecule	MM (g/mol)	bp (^O C)	state at 25 ^o C
NH ₃	17	-33	gas
PH ₃	34		
AsH ₃	78		
SbH ₃	125		
BiH ₃	212		

Continued...

Molecule	MM (g/mol)	bp (^O C)	state at 25 ^o C
OH ₂	18		
SH ₂	34		gas
SeH ₂	81		gas
TeH ₂	130	-2	gas

Molecule	MM (g/mol)	bp (^O C)	state at 25 ^o C
FH	20	+20	gas
CIH	36		
BrH	81		

d. Hydrogen bonding occurs in solutions even when only one of the members can actually hydrogen bond. For example, aqueous methanal (formaldehyde, HCHO): the aldehyde has no hydrogen-bonding H, but it has two lone pairs on oxygen that can participate in H-bonding with water's O-H hydrogens.

C. Instantaneous dipole (London-dispersion) forces (1 – 10 kJ/mol)

A. Strength of the forces: $E \propto \frac{-IE\alpha^2}{r^6}$ where α is the polarizability and IE is the

ionization energy

1. The polarizability increases with MM and shape of the molecule

MM factors: All molecules have MM so all molecules have LDF to some extent.

Molecule	MM (g/mol)	bp (K)	state at 25 ^O C
F ₂	38		
Cl ₂	71		
Br ₂	160		
۱ ₂	254		

Molecule	MM (g/mol)	bp (^O C)	state at 25 ^o C
n-C ₅ H ₁₂	72		
iso-C ₅ H ₁₂	72		
neo-C ₅ H ₁₂	72		

D. lon-dipole forces (10 - 50 kJ/mol)

Only applies to solutions, usually aqueous solutions

For polar molecule: the dipole force is given by

 μ = qr' where q = the equal and opposite charges in the molecule (δ^+ , δ^-) and r' is the distance between δ^+ and δ^- and **e** is the charge on the ion.

For ion-dipole forces,
$$E \propto \frac{\mu e}{r^2}$$



3. Predicting physical states at room temperature.

This chart is overly simplistic, but it shows how LDF can be a very important factor (high MM). In the chart, the MM cut-offs of 100 and 200 g/mol, are rather arbitrary and you can expect to find numerous exceptions.



ММ	Non-polar	Polar A little … A lot	H-bonding A little … A lot
< 100	Gas	Gas liquid	Gas Liquid
100 – 200	Gas or liquid	Gas Liquid	Liquid
200 – 300	Liquid or solid	Liquid Solid	Solid
> 300	Solid	Solid	Solid

1. Use the chart to predict the physical state at room temperature for each of the following. Also, identify which forces led you to your conclusion. In our next class, I will "reveal" the actual melting and boiling points! (Or, if you just can't wait, look them up in a chemistry handbook!)

	Actual mp, bp,
Compound:	phase at room
	temperature
AsBr ₃	
MM = 315 g/mol	
BF ₃	
MM = 68 g/mol	
CSe ₂	
MM = 170 g/mol	
CH ₃ CI	
MM = 50.5 g/mol	
NH ₄ Br	
MM = 98 g/mol	
CCI ₄	
MM = 154 g/mol	
CIO ₂	
MM = 67.5 g/mol	
CIF ₃	
MM = 92.5 g/mol	
Cl ₂ O ₇	
MM = 183 g/mol	
(C ₂ F ₄) _n	
MM = 100 g/mol	
PSCI ₃	
MM = 169.5 g/mol	
PSBr ₃	
MM = 303 g/mol	

SCI ₂ O ₂	
MM = 135 g/mol	
BaCl ₂	
MM = 208 g/mol	
GeBr ₄	
MM = 392 g/mol	
PBr ₃	
MM = 271 g/mol	
C ₂ H ₆ O, ethanol, C ₂ H ₅ OH	
MM = 46 g/mol	
C_2H_6O , dimethylether, CH_3OCH_3	
MM = 46 g/mol	
SiC	
MM = 43 g/mol	
PF ₃	
MM = 88 g/mol	
PF ₅	
MM = 126 g/mol	
PCI ₃	
MM = 137.5 g/mol	
MgO	
MM = 40.3 g/mol	
Fe	
MM = 55.9 g/mol	
(C ₂ H ₅) ₂ NH	
MM = 73 g/mol	
(CH ₃) ₂ NH	
MM = 45 g/mol	
(CH ₃) ₃ N	
MM = 59 g/mol	

Review for ACS Final Exam in Inorganic Chemistry

Intermolecular forces

- 1. Which of these compounds most likely a gas at room temperature?
 - (a) BF₃
 - (b) PBr₃
 - (c) $K_2S_2O_3$
 - (d) SnF₂
 - (e) SiO₂

2. Which of these compounds exhibits hydrogen bonding?

- (a) B₂H₆
- (b) CH₄
- (c) $CH_3CH_2NCI_2$
- (d) CH₃OCI
- (e) HOBr
- 3. Lattice energy is greatest for:
 - (a) NaCl
 - (b) MgO
 - (c) $BaCl_2$
 - (d) Na₂O
 - (e) CsF
- 4. Identify the species with the highest melting point.
 - (a) AsCl₃
 - (b) $NH_4C_2H_3O_2$
 - (c) SiC
 - (d) Mn
 - (e) S₈

Answers: A, E, B, C

Day 3 answers:

2 groups	name	sketch	angles	example
AB ₂	linear	В — А — В	180 ^o	CO ₂
				SCN ⁻
ABE	(none)	В — А :	not applicable	CN-

2. Geometries and their name and angles

3 groups	name	sketch	angles	example
AB ₃	trigonal plane	B B B B B	120 ^o	ВF ₃ CO ₃ ²⁻
AB ₂ E	bent	B A B	~ < 120 ^o	NO2⁻
ABE ₂	(none)	B — A.	not applicable	NO

4 groups	name	sketch	angles	example
AB ₄	tetrahedral	B	109.5 ^o	CH ₄
		B A B		SO ₄ 2-
AB ₃ E	trigonal pyramid	B B B B	~ < 109.5 ^o	NH ₃ SO ₃ 2-
AB ₂ E ₂	bent	B B B	~ < 109.5 ^o	OH ₂ CIO ₂ -
ABE3	(none)	в—А:	not applicable	HCI

3. Expanding octets:

O groupsnamenamename AB_5 trigonal bipyramid $B_{B} \rightarrow A_{B} = B_{B}$ 120° 180° PF_5 AB_4E see-saw $B_{B} \rightarrow A_{B} = B_{B}$ $2 < 0^{\circ}$ 180° SF_4 SbF_3^{-1} AB_3E_2 T-shaped $B_{B} \rightarrow A_{B} = B_{B}$ $B \rightarrow A_{B} = B_{B}$ $\sim < 90^{\circ}$ $\sim < 180^{\circ}$ SF_3^{-1} AB_3E_2 T-shaped $B_{B} \rightarrow A_{B} = B_{B}$ $B \rightarrow A_{B} = B_{B}$ 180° SF_3^{-1} AB_2E_3 linear $B_{B} \rightarrow A_{B} = B_{B}$ 180° XeF_2 IF_2^{-1} $B_{B} \rightarrow A_{B} = B_{B}$ 00° $B \rightarrow A_{B} = B_{B}$ SF_6 SF_6 PF_6^{-1} AB_5E square pyramid $B_{B} \rightarrow A_{B} = B_{B}$ 90° SF_6 SF_6 SF_6 AB_4E_2 square plane $B_{B} \rightarrow A_{B} = B_{B}$ 90° SF_6 XeF_4 180° AB_7 name pentagonal bioyramid $Sketch$ $B \rightarrow B$ angles $B \rightarrow B$ example SR_6 B_7 name pentagonal bioyramid $Sketch$ $B \rightarrow B$ angles $R \rightarrow B$ example B_7 name pentagonal bioyramid $Sketch$ $B \rightarrow B$ angles $R \rightarrow B$ example B_7 name $R \rightarrow B$ $Snuare$ antiorism Se_7 Se_7	5 groups	name	sketch	angles	example
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AB _o Square antiprism XeF _o	8 groups	name	sketch	angles	example
	AB ₈	Square antiprism	$\langle \rangle$		XeF ₈
			$\mathbf{\mathbf{X}}$		

Step 5:

PCl ₄ + AB ₄	$PCI_5 AB_5$
SF ₄ AB ₄ E	$CIF_3 AB_3E_2$
IO ₄ - AB ₄	BrO ₃ - AB ₃ E
SF ₄ O AB ₅	ClO ₂ F ₃ AB ₅
	PCI ₄ + AB ₄ SF ₄ AB ₄ E IO ₄ - AB ₄ SF ₄ O AB ₅

4. On bulkiness of electrons and bonding groups

(See 2 above: Geometries and their name and angles for details about angles)

PCl ₃ AB ₃ E	$SCI_2 AB_2E_2$	ОН ₃ + АВ ₃ Е
BrF ₅ AB ₅ E	$SF_4 AB_4E$	CH ₃ ⁻AB ₃ E

For species with 5 structural groups. (See 2 above: Geometries and their name and angles for details about angles)

SbF ₄ ⁻ AB ₄ E	CIF3 AB3E2	ICI ₄ + AB ₄ E
PCI ₅ AB ₅	SF ₄ AB ₄ E	ICI2 ⁻ AB2E3

Similarly, for species with 5 structural groups, oxygen groups prefer the equatorial positions. Oxygen atoms and E-groups always go equatorial! (See 2 above: Geometries and their name and angles for details about angles)

SF ₄ O AB ₅	CIO ₂ F3 AB5	SeF ₃ O⁻ AB ₄ E
SeF ₃ O ₂ - AB ₅	IF₂O₃ ⁻ AB₅	

5. On formal charge and bond order (BO)



6. On resonance

SO ₂ 2 resonance forms that obey octet, plus one drawing that minimizes FC, but places 10 electrons around S.	SO ₄ -2 1 form that obeys octet, plus 6 drawings, each with 2 SO double bonds, that minimize FC, but places 12 electrons around S. No structures should have more than 2 dbl bonds.	SO ₃ ⁻² 1 form that obeys octet, plus 3 drawings, each with one SO double bond, that minimize FC, but places 10 electrons around S. No structures should have more than 1 dbl bond.
NO ₃ ⁻ Three resonance forms, all of which obey the octet rule	PO ₄ ⁻³ 1 form that obeys octet, plus 4 drawings, each with one PO double bond, that minimizes FC, but places 10 electrons around P. No structures should have more than 1 dbl bond.	SbF ₄ - One Lewis dot structure
XeO ₄ 1 form that obeys octet, plus 1 drawing with 4 XeO double bonds, that minimizes FC, but places 16 electrons around Xe. The latter is quite unlikely.	ClO ₂ - 1 form that obeys octet, plus 2 drawings, each with one ClO double bond, that minimizes FC, but places 10 electrons around Cl. No structures should have more than 1 dbl bond.	CO ₃ ⁻² Three resonance forms, all of which obey the octet rule

7. On paramagnetic substances.



8. On polarity.

SO ₂ , polar	SO ₃ , non-polar	SF ₄ , polar
SF ₆ , non-polar	SF ₄ O, polar	SO ₂ Cl ₂ , polar
XeO ₄ , non-polar	ClO ₂ , polar	PF ₅ , non-polar

9. On subvalent central atom species

