



## Homework 2

(0.8') 1. In a gaseous KCl molecule, the internuclear distance is  $2.67 \times 10^{-10}$  m. Using data from Appendix F and neglecting the small, short-range repulsion between the ion cores of  $K^+$  and  $Cl^-$ , estimate the dissociation energy of gaseous KCl into K and Cl atoms (in  $\text{kJ mol}^{-1}$ ).

该过程分两步：a. 离子键断裂  $KCl \rightarrow K^+ + Cl^-$ ，b.  $Cl^-$  中多余的电子迁移到  $K^+$  中

$$E_a = -N_A \times Q_1 Q_2 / 4\pi\epsilon r = 520 \text{ kJ/mol (需要 520 kJ/mol 的能量)}$$

$$E_b = \text{Cl 的亲和能} - \text{K 的电离能} = 349.0 - 418.8 = -69.8 \text{ kJ/mol (吸收 69.8 kJ/mol)}$$

$$\therefore E = E_a + E_b = 450.2 \text{ kJ/mol (需要 450.2 kJ/mol)}$$

知道  $E = E_a + E_b$  以及  $E_a$ 、 $E_b$  的计算方法各得 0.2 分

(0.6') 2. Estimate the percent ionic character of the bond in each of the following diatomic molecules, based on the dipole moment.

	Bond Length (Å)	Dipole Moment (D)
ClO	1.573	1.239
KI	3.051	10.82
TiCl	2.488	4.543
InCl	2.404	3.79

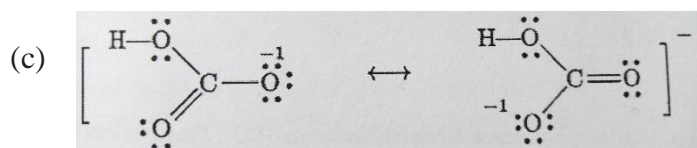
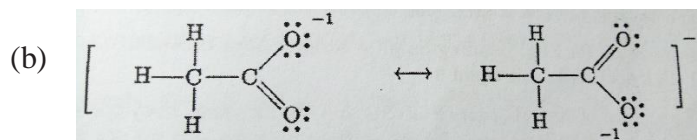
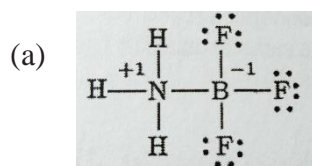
$$\text{双原子分子离子性百分数 } \delta = 0.2082 \mu / r$$

$$\delta_{\text{ClO}} = 0.16 \quad \delta_{\text{KI}} = 0.74 \quad \delta_{\text{TiCl}} = 0.38 \quad \delta_{\text{InCl}} = 0.33$$

知道计算方法得 0.4 分，每处计算错误扣 0.05 分

(0.6') 3. Draw Lewis electron dot diagrams for the following species, indicating formal charges and resonance diagrams where applicable.

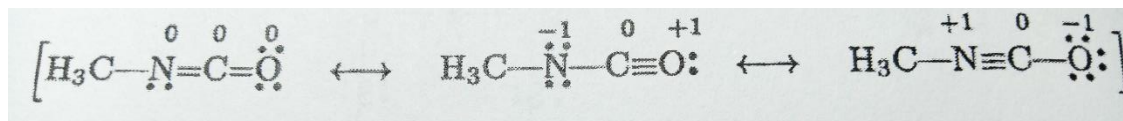
(a)  $\text{H}_3\text{NBF}_3$       (b)  $\text{CH}_3\text{COO}^-$  (acetate ion)      (c)  $\text{HCO}_3^-$  (hydrogen carbonate ion)



每问 0.2 分



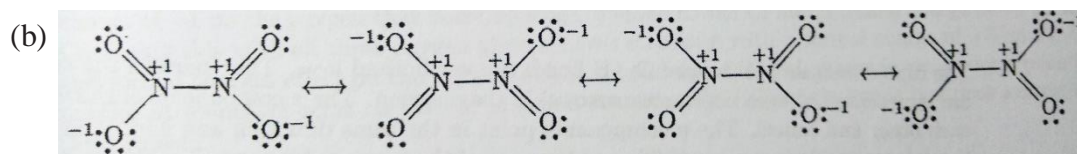
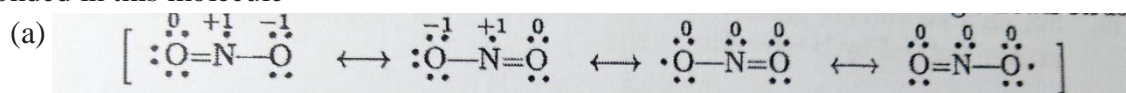
(0.6') 4. Methyl isocyanate, which was involved in the disaster in Bhopal, India, in 1984, has the chemical formula  $\text{CH}_3\text{NCO}$ . Draw its Lewis diagram, including resonance forms. (Note: The N atom is bonded to the two C atoms.)



(0.8') 5. The two compounds nitrogen dioxide and dinitrogen tetroxide are introduced in Section 3.13.

(a)  $\text{NO}_2$  is an odd-electron compound. Draw the best Lewis diagrams possible for it, recognizing that one atom cannot achieve an octet configuration. Use formal charges to decide whether that should be the (central) nitrogen atom or one of the oxygen atoms.

(b) Draw resonance forms for  $\text{N}_2\text{O}_4$  that obey the octet rule. The two N atoms are bonded in this molecule



每问 0.4 分

(0.6') 6. (a) Predict the geometry of the  $\text{SbCl}_5^{2-}$  ion, using the VSEPR method.

(b) The ion  $\text{SbCl}_6^{3-}$  is prepared from  $\text{SbCl}_5^{2-}$  by treatment with  $\text{Cl}^-$ . Determine the steric number of the central antimony atom in this ion, and discuss the extension of the VSEPR theory that would be needed for the prediction of its molecular geometry.

(a)  $\text{SN}=5+1=6$ ，为四角锥

(b) 对于 Sb 来说，成键电子对数+1，孤对电子数不变，故  $\text{SN}=7$

VSEPR 理论需要扩展到  $\text{SN}=7$  的情况才能预测该结构

第一问算出 SN 与答出构型各得 0.2 分，第二问 0.2 分