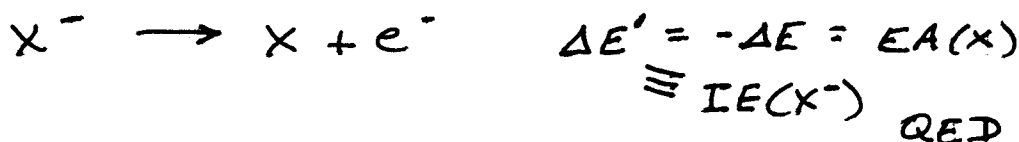


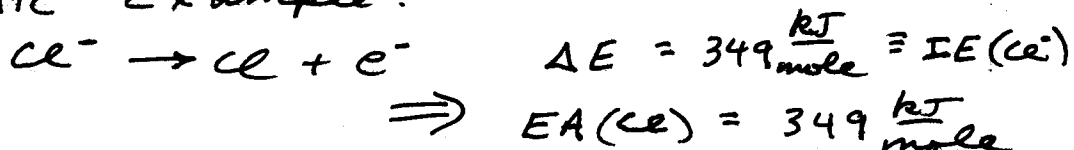
LECTURE # 6, Wednes., 10/12

\* Finish estimate of  $\Delta E_d$  for  $K^+F^-$   
 (see last page of LECTURE #5)

\* Discuss further, IE's and EA's  
 E.g.,  $EA(X) = IE(X^-)$



Specific example:



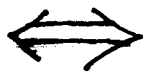
HALOGEN ATOMS HAVE HIGH EA'S FOR SAME REASON THAT NOBLE GAS ATOMS HAVE HIGH IE'S

Note that  $IE(X^-) \ll IE(X) \\ \Rightarrow EA(X) \ll IE(X)$

\* <sup>Electron</sup> EN's

upper right corner

(high IE's  
high EA's)



hard to remove  $e^-$   
easy to add  $e^-$

$e^-$  "acceptor"

"electronegative"

i.e., high EN,  $\propto (IE + EA)$

OPPOSITE IS TRUE FOR (ELECTROPOS.) ELEMENTS  
 IN LOWER LEFT CORNER

## \* PARTIAL IONIC CHARACTER

\* Preceding estimate of KF binding energy is approximate for many reasons, one of which is that the bond is not completely ionic, i.e., there is not quite a complete transfer of an electron from K to F.

### DIGRESSION: DIPOLE MOMENTS


→ dipole moment is <sup>the</sup> a measure of charge separation in a molecule (or any other distribution of charge)

E.g., He, H<sub>2</sub>, Cl<sub>2</sub>, ... have no dipole moment

But HF, KF, H<sub>2</sub>O, ... do

→ DEFINITION: charges  $-Q$  and  $+Q$  separated by distance  $R$ , have a dipole moment of  $QR \equiv \mu$

E.g.,  $(+e) \xrightarrow{1.0\text{\AA}} (-e) \Rightarrow \mu = (1.6 \times 10^{-19} \text{ C})(1.0 \times 10^{-10} \text{ m})$   
 $= 1.6 \times 10^{-29} \text{ C m}$

In HCl, ~~one~~  one measures a dipole moment of  $3.7 \times 10^{-30} \text{ C m}$

For CO,  $\mu = 0.37 \times 10^{-30} \text{ C m}$

For KCl,  $\mu = 34.4 \times 10^{-30} \text{ C m}$ , etc.

→ So it's natural to agree on some intermediate/typical  $\mu$  as our unit of dipole moment:

$$1 \text{ Debye} \equiv 3.336 \times 10^{-30} \text{ C m}$$

E.g.,  $\mu = \begin{matrix} 1.1 \text{ D} \\ 0.1 \text{ D} \\ 10.3 \text{ D} \end{matrix}$  for  $\begin{matrix} \text{HCl} \\ \text{CO} \\ \text{KCl} \end{matrix}$

\* Let's go back to our model of KF as a perfect ionic bond ( $\rightarrow$  complete transfer of one electron from K to F)

$R = 2.17 \text{ \AA}$  and complete e transfer ( $\Rightarrow$   $+e$  and  $-e$  separated by  $2.17 \text{ \AA}$ ) would imply

$$\begin{aligned} \mu_{KF} &= eR = (1.60 \times 10^{-19} \text{ C}) (2.17 \times 10^{-10} \text{ m}) \\ &= 34.7 \times 10^{-30} \text{ C m} \\ &= \frac{34.7 \times 10^{-30} \text{ C m}}{3.34 \times 10^{-30} \text{ C m/D}} = 10.4 \text{ D} \end{aligned}$$

But measured  $\mu$  (and  $R$ ) is  $8.6 \text{ D}$   
(and  $R = 2.17 \text{ \AA}$ )

Thus, instead of charge  $+e$  &  $-e$  at each end of molecule, we must have  $\pm \frac{8.6}{10.4} e$  at each end:  $\pm 0.83 e$

"BOND IS 83% IONIC"

$\rightarrow$  This is one of the reasons our estimate of bond energy was too big (since Coulomb attraction interaction energy  $\propto Q_{\text{eff}}^2$ )

\* COVALENT BONDS (vs IONIC)

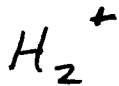
	$R_e$	$\Delta E_d$
HF	$0.926 \text{ \AA}$	$565 \frac{\text{kJ}}{\text{mole}}$
HCl	$1.284$	$429$
HBr	$1.424$	$363$
HI	$1.620$	$295$

$\rightarrow$  atomic sizes also increase in this order  
 $\rightarrow$  bond lengths and energies are approximately constant (for given pair of bonded atoms) from one compound to another

	BOND ORDER	$R_e$	$\Delta E_d$ $\frac{\text{kJ}}{\text{mole}}$
single	C-C ethane	1.536 Å	345
double	C=C ethylene	1.337	612
triple	C≡C acetylene	1.204	809

Similarly, with  
 N-N, N=N, N≡N  
 C-O, C=O  
 N-O, N=O

\* COVALENT BOND AS SHARED  $e^-$  PAIR



$R_e = 1.06 \text{ Å}, \quad \Delta E_d = 255 \frac{\text{kJ}}{\text{mole}}$

$H_2$  has 2  $e^-$ 's in middle (shared)

$R_e = 0.75 \text{ Å}, \quad \Delta E_d = 433 \frac{\text{kJ}}{\text{mole}}$