

1

Bond

Get  $\Delta$ -Dissociation Energy from Heat of Formation  
BDE or  $D_0$

$$\text{e.g. } \text{H}_2 \rightarrow D_0 = 104 \text{ kcal/mol} \\ = 436 \text{ kJ/mol}$$

$$N_{\text{Avogadro}} = 6.02214179 \times 10^{23} \text{ mol}^{-1} \\ 1 \text{ kJ} = \frac{10^3}{1.602 \times 10^{-19}} = 6.24150974 \times 10^{21} \text{ eV}$$

$$\Rightarrow 1 \text{ kJ/mol} = \frac{6.24 \times 10^{21}}{6.022 \times 10^{23}} \text{ eV (per molecule)} \\ = 0.01036427 \text{ eV}$$

$$\Rightarrow 436 \text{ kJ/mol} \rightarrow 4.5188 \text{ eV} \quad \text{seems to be correct modern number}$$

$$\text{In Huber & Herzberg } D_0 = 4.55632 \text{ eV}$$

Standard enthalpy of formation

Can get this from Heats of Formation of components

$$\Rightarrow \Delta_f H_{\text{gas}}^\circ (\text{H}) = 217.998 \pm 0.006 \text{ kJ/mol}$$



$$\Delta H_{\text{reaction}}^\circ = \sum \Delta H_f^\circ (\text{products}) - \sum \Delta H_f^\circ (\text{reactants})$$



2.

All elements in their standard states (e.g.  $H_2$  gas)  
have  $\Delta H_f^\circ = 0$

So for dissociation  $H_2 \rightarrow H+H$

$$\begin{aligned}\Delta H_{\text{dissociation}}^\circ &= 2 \times 218 - 0 \\ &= +436 \text{ kJ/mol}\end{aligned}$$

five  $\Rightarrow$  endo-thermic as expected.

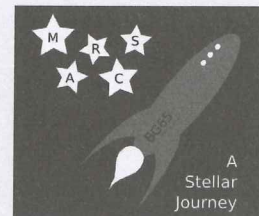
Standard states

liquids :  $H_2, Br_2$

gases :  $He, Ne, Ar, Kr, Xe, Rn$

+  $H_2, O_2, N_2$

solid : all others.



eg. II CH  $D_0 = 410 \text{ kJ/mol}$   
 $= 4.25 \text{ eV}$   
 Huber & Herzberg  $\Rightarrow 3.465 \text{ eV}$  !

This is some 3.  
 kind of average  
 of C-H bond  
 in molecules i.e.  
 including polyatomic

$$\Delta H_f^\circ \text{ gas}$$

C	=	$716.68 \pm 0.45$	$\text{kJ/mol}$
H	=	$217.988 \pm 0.006$	
CH	=	$594.13 \pm$	

$$\Rightarrow \Delta H^\circ \text{ dissociation} = 717 + 218 - 594$$

$$= 341$$

$$\Rightarrow 3.53 \text{ eV.}$$

See Lange's Hand book

specifically C-H  $\Rightarrow D_0 = 337.2(8) \text{ kJ/mol}$   
 $= 3.49 \text{ eV} \checkmark$

But note, all sources, pre 1966.



4.

as III  $\text{TiO}$

$$\text{H\&H} \rightarrow D_0^\circ = 6.87 \text{ eV}$$

$\Delta_f H^\circ_{\text{gas}}$

$$\text{Ti} \rightarrow 473 \pm 3$$

$$\text{O} \rightarrow 249.18 \pm 0.1$$

$$\text{TiO} \rightarrow 54.39$$



$$\Delta H^\circ = 473 + 249 - 54$$

$$= 668$$

$$\Rightarrow 6.92 \text{ eV} \quad \left( \text{c.f. Lange } 662(16) \right. \\ \left. \text{agrees within error} \right) \\ \Rightarrow 6.86 \text{ eV.}$$

Problem Most data for  $\Delta_f H$  is from Chase 1998, NIST-JANAF Thermochemical tables, and data was often last reviewed in Dec 1973.

The atomic values seen to generally have been reviewed in Cox, Wagman et al 1984. (CODATA)