Bond

Get Dissociation Energy from Heat of Formation

BDE or D_0

e.g. $H_2 \rightarrow$ $D_0 = 104$ kcal/mol

$= 436$ kJ/mol

$N_{Avagadro} = 6.022\,141\,79 \times 10^{23}$ mol^{-1}

$1\ kJ = \frac{10^3}{1.602 \times 10^{-19}} = 6.241\,509\,74 \times 10^{21}$ eV

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

$= 0.010364\,27$ eV

$\Rightarrow 436$ kJ/mol $\longrightarrow$ 4.5188 eV

seems to be correct modern number

In Huber & Herzberg $D_0 = 4.55632$ eV

Can get this from Heats of Formation of components

Standard enthalpy of formation

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

$H_2 \longrightarrow H + H$

$\Delta H^\circ_{reaction} = \Sigma\ \Delta H_f^\circ(products) - \Sigma\ \Delta H_f^\circ(reactants)$

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

So for dissociation $H_2 \rightarrow H + H$

$$\Delta H^\circ_{dissociation} = 2 \times 218 - 0$$
$$= +436 \text{ kJ/mol}$$

+ive $\Rightarrow$ endo-thermic as expected.

Standard states

liquids : Hg_2, Br_2

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

+ H_2, O_2, N_2

solid : all others.

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A Stellar Journey

eg. II CH D_0 = 410 kJ/mol = 4.25 eV } This is some kind of average of C-H bond in molecules i.e including polyatomic ?

Huber & Herzberg ⇒ 3.465 eV !

ΔH_f° gas C = 716.68 ± 0.45 kJ/mol

H = 217.998 ± 0.006

CH = 594.13 ±

$\Rightarrow \Delta H^\circ_{dissociation}$ = 717 + 218 − 594

= 341

⇒ 3.53 eV.

See Lange's Handbook

specifically C−H ⇒ D_0 = 337.2(8) kJ/mol)

⇒ 3.49 eV ✓

But note, all sources, pre 1966.

es III TiO

$H\&H \rightarrow D_0^\circ = 6.87$ eV

$\Delta_f H^\circ_{gas}$

Ti	$\rightarrow$ 473	± 3
O	$\rightarrow$ 249.18	± 0.1
TiO	$\rightarrow$ 54.39	

$TiO \rightarrow Ti + O$

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

$= 668$ (c.f. Lange 662(16) agrees within error)

$\Rightarrow 6.92$ eV $\Rightarrow 6.86$ 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 seem to generally have been reviewed in Cox, Wagman etal 1984 (CODATA)