

Chemistry 163B Winter 2013

Lectures 6-7 Thermochemistry

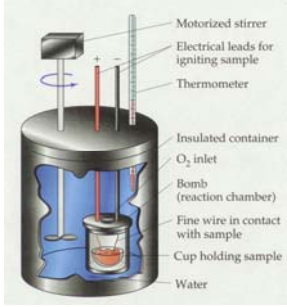
Chemistry 163B
Thermochemistry
Chapter 4 Engel & Reid

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heats of reactions (constant volume; 'bomb' calorimeter)

$$\Delta U_V = q_V$$

$$\Delta U = U_{\text{products}} - U_{\text{reactants}}$$

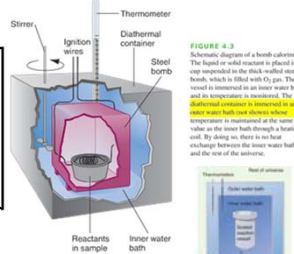


4

heats of reactions (constant volume; fig 4.3 E&R)

$$\Delta U_V = q_V$$

$$\Delta U = U_{\text{products}} - U_{\text{reactants}}$$

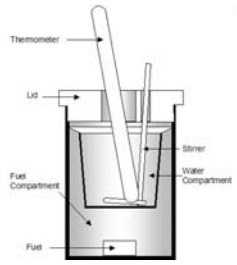


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heats of reactions (constant pressure; 'coffee cup calorimeter')

$$\Delta H_P = q_P$$

$$\Delta H = H_{\text{products}} - H_{\text{reactants}}$$

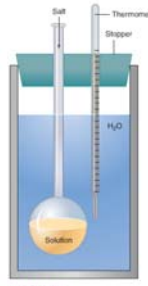


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heats of reactions (constant pressure; fig 4.4 E&R)

$$\Delta H_P = q_P$$

$$\Delta H = H_{\text{products}} - H_{\text{reactants}}$$



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most reactions at P constant, $\Delta H_P = q_P$

$$\text{C}(\text{gr}) + \text{O}_2(\text{g}) \rightarrow \text{CO}_2(\text{g}) \quad \Delta H_{298} = -393 \text{ kJ}$$

$$\text{ATP} + \text{H}_2\text{O} \rightarrow \text{ADP} + \text{H}_3\text{PO}_4 \quad \Delta H_{298} \approx -20.5 \text{ kJ}$$

$$\text{SiO}_2 (\alpha \text{ quartz}) \rightarrow \text{SiO}_2 (\beta \text{ quartz}) \quad \Delta H_{848} = -907 \text{ kJ}$$

$$\text{NaCl}(\text{s}) + \text{H}_2\text{O} (\ell) \rightarrow \text{Na}^+(\text{aq}) + \text{Cl}^-(\text{aq}) \quad \Delta H_{298} = +3.9 \text{ kJ}$$

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Lectures 6-7 Thermochemistry

topics for thermochemistry, parts of Ch. 4 Engel & Reid

- HW#3 16,17,18** • Calculate $\Delta H_{\text{reaction}}$
Hess's Law, standard heats of formation
- HW#3 16** • $\Delta H_{\text{reaction}}$ vs $\Delta U_{\text{reaction}}$
- HW#3 18, *19** • Temperature (and later pressure) dependence of $\Delta H_{\text{reaction}}$
- Calorimetry
- HW#3 20, 21** • Heats of solution
- $\Delta H_{\text{reaction}}$ from bond enthalpies

----- MIDTERM 1 ----- 9

Hess's Law

$$\Delta H_{\text{reaction}} = H_{\text{products}} - H_{\text{reactants}}$$

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ΔH State Function \Rightarrow Hess's Law

ΔH kJ		ΔH kJ
ΔH_{I}	$\text{C}(\text{gr}) \rightarrow \text{C}(\text{dia})$?
ΔH_{II}	$\text{C}(\text{gr}) + \text{O}_2(\text{g}) \rightarrow \text{CO}_2(\text{g})$	-393.51
ΔH_{III}	$\text{CO}_2(\text{g}) \rightarrow \text{C}(\text{dia}) + \text{O}_2(\text{g})$	+395.41
$\Delta H_{\text{I}} = \Delta H_{\text{II}} + \Delta H_{\text{III}} = 1.90 \text{ kJ}$		

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factors affecting $\Delta H_{\text{reaction}}$

- stoichiometry
 ΔH is extensive; $\Delta \bar{H}$ is intensive
- physical state
phase or crystal form of reactants and products
- temperature and pressure
- does **NOT** depend on path

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notation: ΔH (etc) in terms of molar enthalpies and stoichiometric coefficients

$$n_A A + n_B B \rightarrow n_C C + n_D D \quad \Delta H_{\text{reaction}} = n_C \bar{H}_C + n_D \bar{H}_D - n_A \bar{H}_A - n_B \bar{H}_B$$

$$H_{\text{prods}} = \sum_{i=\text{prods}} n_i \bar{H}_i$$

$$H_{\text{reacts}} = \sum_{i=\text{reacts}} n_i \bar{H}_i$$

$\Delta H_{\text{reaction}} = \sum_{i=\text{prods}} n_i \bar{H}_i - \sum_{i=\text{reacts}} n_i \bar{H}_i$

$\Delta H_{\text{reaction}} = \sum_i v_i \bar{H}_i$

v_i is stoichiometric coefficient of i^{th} reactant / product

$v_i = n_i$ if i is product species

$v_i = -n_i$ if i is reactant species

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$\Delta H_{\text{reaction}}$ vs $\Delta U_{\text{reaction}}$ at fixed temperature T

$$H \equiv U + PV$$

$$\Delta H = H_{\text{prods}} - H_{\text{reacts}}$$

$$\Delta H = \Delta U + \Delta(PV) = \Delta U + (PV)_{\text{prods}} - (PV)_{\text{reacts}}$$

assume:

- i) PV and ΔPV is small for solids and liquids
- ii) Gasses follow ideal gas law

$$\Delta PV = (PV)_{\text{prods}} - (PV)_{\text{reacts}}$$

$$\Delta PV = (n_{\text{gas}} R)_{\text{prod}} - (n_{\text{gas}} R)_{\text{react}}$$

$$\Delta PV = \Delta n_{\text{gas}} RT$$

$$\Delta H_{\text{reaction}} = \Delta U_{\text{reaction}} + \Delta n_{\text{gas}} RT$$

E&R eqn 4.25

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standard states and enthalpies of formation (done on board)

standard state

$\Delta H^\circ(T, P = 1 \text{ atm [or 1 bar]})$

often T is assumed 298K for standard state ΔH°_{298}

define standard states \Rightarrow

$(\Delta \bar{H}^\circ_{298})_{\text{formation}} \equiv \bar{H}_f^\circ$ ← molar enthalpy of formation

define enthalpy of formation \Rightarrow

ΔH°_{298}

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$\Delta H^\circ_{\text{rxn}}$ from H_f°

reactants \rightarrow products

$(-\Delta H_f^\circ)_{\text{reactants}}$ $(\Delta H_f^\circ)_{\text{products}}$

elements in most stable state

$(\Delta H^\circ)_{\text{rxn}} = \sum_i \nu_i (\bar{H}_f^\circ)_i$

do HW#3 problem 16b (E&R 4.20b)

$\Delta H^\circ_{\text{rxn}}$

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topics for thermochemistry, parts of Ch. 4 E&R

- ✓ Calculate $\Delta H_{\text{reaction}}$
Hess's Law, standard heats of formation
- ✓ $\Delta H_{\text{reaction}}$ vs $\Delta U_{\text{reaction}}$
- Temperature (and pressure) dependence of $\Delta H_{\text{reaction}}$
- Calorimetry
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----- MIDTERM 1 -----

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temperature dependence of H of substance at constant P

change in enthalpy of substance $T_1 \rightarrow T_2$

$dH = n\bar{C}_p dT + \left(\frac{\partial H}{\partial P}\right)_T dP$

for a given reactant or product at constant P

$dH_p = n\bar{C}_p dT \quad d\bar{H}_p = \bar{C}_p dT$

$\int_{T_1}^{T_2} d\bar{H} = \int_{T_1}^{T_2} \bar{C}_p dT$

$\bar{H}(T_2) - \bar{H}(T_1) = \int_{T_1}^{T_2} \bar{C}_p dT$

$\bar{H}(T_2) = \bar{H}(T_1) + \int_{T_1}^{T_2} \bar{C}_p dT$

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temperature dependence of $\Delta H_{\text{reaction}}$ (reaction carried out at constant P, T)

$\Delta H_{\text{reaction}} = \sum_i \nu_i \bar{H}_i$

$\bar{H}_i(T_2) = \bar{H}_i(T_1) + \int_{T_1}^{T_2} \bar{C}_{p,i} dT$

$\Delta H_{\text{reaction}}(T_2) = \sum_i \nu_i \bar{H}_i(T_2)$

$\Delta H_{\text{reaction}}(T_2) = \sum_j \nu_j \bar{H}_j(T_1) + \sum_i \nu_i \int_{T_1}^{T_2} \bar{C}_{p,i} dT$

$\Delta H_{\text{reaction}}(T_2) = \Delta H_{\text{reaction}}(T_1) + \int_{T_1}^{T_2} \Delta C_p dT$

change of ΔH_{rxn} $T_1 \rightarrow T_2$

where $\Delta C_p = \sum_i \nu_i (\bar{C}_p)_i = "(C_p)_{\text{products}} - (C_p)_{\text{reactants}}"$

$\Delta H_{\text{rxn}}(T_1, P)$

vs

$\Delta H_{\text{rxn}}(T_2, P)$

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example problems : ΔH from H_f° and ΔH T=298K \rightarrow 398K

$3\text{C}_2\text{H}_2(\text{g}) \rightarrow \text{C}_6\text{H}_6(\ell)$ calc ΔH°_{298}

$(\Delta \bar{H}_f^\circ)_{298}$ 227.4 49.1 kJ mol^{-1}

$(\Delta H^\circ)_{298} = -3(227.4) + 1(49.1) = -633.1 \text{ kJ [per mol C}_6\text{H}_6(\ell)]$

$(\text{mol})(\text{kJ mol}^{-1}) + (\text{mol})(\text{kJ mol}^{-1}) = \text{kJ}$

$3\text{C}_2\text{H}_2(\text{g}) \rightarrow \text{C}_6\text{H}_6(\ell)$ calc ΔH°_{398}

\bar{C}_p 44. 136.0 $(\text{J K}^{-1} \text{ mol}^{-1})$

$\Delta \bar{C}_p$ -3(44.0) + 1(136.0) = 4.0 (J K^{-1})

$(\Delta H^\circ)_{398} = (\Delta H^\circ)_{298} + \int_{298}^{398} \Delta C_p dT = (\Delta H^\circ)_{298} + \Delta C_p \Delta T$ C_p independent of T

$(\Delta H^\circ)_{398} = -633.1 \text{ kJ} + (4.0 \times 10^{-3} \text{ kJ K}^{-1})(100\text{K}) = -632.7 \text{ kJ}$

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topics for thermochemistry, parts of Ch. 4 E&R

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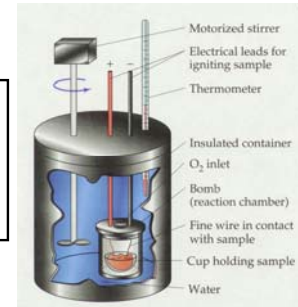
MIDTERM 1

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heats of reactions (constant volume)

$$\Delta U_v = q_v$$

$$\Delta U = U_{\text{products}} - U_{\text{reactants}}$$

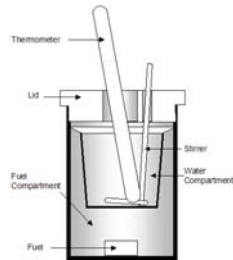


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heats of reactions (constant pressure)

$$\Delta H_p = q_p$$

$$\Delta H = H_{\text{products}} - H_{\text{reactants}}$$



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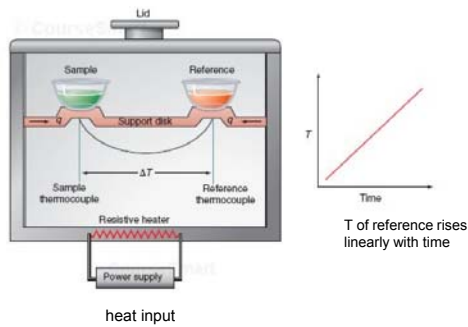
DSC- differential scanning calorimetry (enrichment, don't FRET)



useful for small samples (often biological)

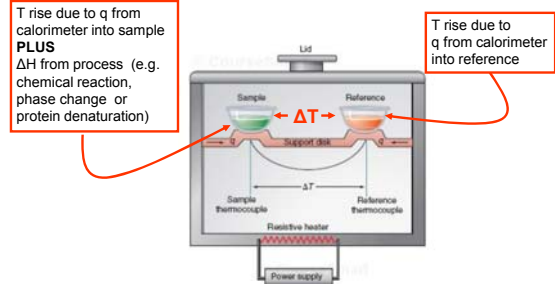
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DTA differential thermal analysis DSC differential scanning calorimetry



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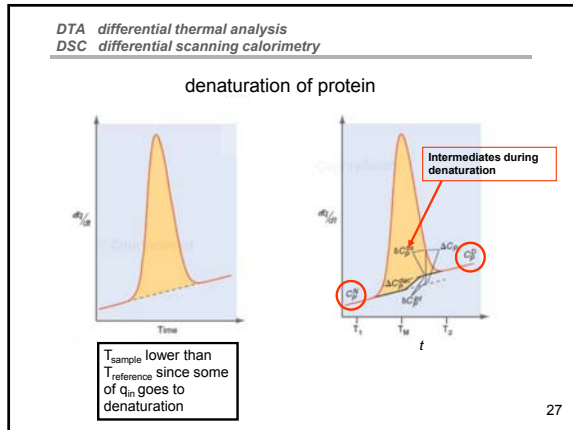
DTA differential thermal analysis DSC differential scanning calorimetry



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how H and ΔH change with pressure (don't FRET now)

will prove later:

$$\left(\frac{\partial \bar{H}}{\partial P}\right)_T = \bar{V} - T \left(\frac{\partial \bar{V}}{\partial T}\right)_P = \bar{V} - T\bar{V}\alpha$$

$$\alpha = \frac{1}{\bar{V}} \left(\frac{\partial \bar{V}}{\partial T}\right)_P \text{ the coefficient of thermal expansion}$$

$$\left(\frac{\partial \Delta H_{\text{reaction}}}{\partial P}\right)_T = \sum_i \nu_i (\bar{V}_i - T\bar{V}_i \alpha_i)$$

Will show later:

dependence of $\Delta H_{\text{reaction}}$ on pressure is usually weak

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heats of formation of ions (heat of solutions), Example 4.4 p 73

importance: how to assign \bar{H}_f^0 for an individual ion in solution since ions come in 'pairs'

resolution: assign $\bar{H}_f^0(\text{H}^+(\text{aq}, 1\text{M})_{\text{ideal}}) = 0$ and measure \bar{H}_f^0 for other ions relative to H^+

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heats of formation of ions (heat of solutions)

HOW TO GET \bar{H}_f^0 for $\text{Cl}^-(\text{aq})$

$$\text{HCl}(g, 1 \text{ bar}) \xrightarrow{-H_2O} \text{H}^+(\text{aq}, 1\text{M})_{\text{ideal}} + \text{Cl}^-(\text{aq}, 1\text{M})_{\text{ideal}}$$

$$\Delta H_{\text{measured}} = -74.9 \text{ kJ}$$

$$-74.9 \text{ kJ} = -\bar{H}_f^0(\text{HCl}(g)) + \bar{H}_f^0(\text{H}^+(\text{aq})) + \bar{H}_f^0(\text{Cl}^-(\text{aq}))$$

$$-74.9 \text{ kJ} = -(-92.3 \text{ kJ}) + 0 + \bar{H}_f^0(\text{Cl}^-(\text{aq}))$$

$$\bar{H}_f^0(\text{Cl}^-(\text{aq})) = -167.2 \text{ kJ mol}^{-1}$$

GOT \bar{H}_f^0 for $\text{Cl}^-(\text{aq})$ NOW

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heats of formation of ions (heat of solutions)

GET \bar{H}_f^0 for $\text{Na}^+(\text{aq})$

$$\text{NaCl}(s) \xrightarrow{-H_2O} \text{Na}^+(\text{aq}, 1\text{M})_{\text{ideal}} + \text{Cl}^-(\text{aq}, 1\text{M})_{\text{ideal}}$$

$$\Delta H_{\text{measured}} = +3.89 \text{ kJ}$$

$$+3.89 \text{ kJ} = -\bar{H}_f^0(\text{NaCl}(s)) + \bar{H}_f^0(\text{Na}^+(\text{aq})) + \bar{H}_f^0(\text{Cl}^-(\text{aq}))$$

$$+3.89 \text{ kJ} = -(-411.2 \text{ kJ}) + \bar{H}_f^0(\text{Na}^+(\text{aq})) + (-167.2 \text{ kJ})$$

$$\bar{H}_f^0(\text{Na}^+(\text{aq})) = -240.1 \text{ kJ mol}^{-1}$$

Substance	ΔH_f^0 (kJ mol ⁻¹)
$\text{Al}^{3+}(\text{aq})$	-538.4
$\text{Ba}^{2+}(\text{aq})$	-537.6
$\text{Br}^-(\text{aq})$	-121.6

etc.

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$\Delta H_{\text{reaction}}$ from bond enthalpies (p. 69)

reactants $\xrightarrow{\Delta H_{\text{reaction}}}$ products

ΔH_{vap} ΔH_{sublim} $-\Delta H_{\text{vap}}$ $-\Delta H_{\text{sublim}}$

reactants (gas phase) $\xrightarrow{\sim \Delta H_{\text{bond enthalpies}}}$ products (gas phase)

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$\Delta H_{\text{reaction}}$ from bond enthalpies

- Similar bonds (C-H, C-C, C=C, C=O, etc) in similar molecule have similar enthalpies (energies)
- Use bond enthalpies (averaged over experimental data from several molecules) to approximate the enthalpies of the bonds broken in reactants and bonds formed in products to approximate **gas phase** $\Delta H_{\text{reaction}}$

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$\Delta H_{\text{reaction}}$ from bond enthalpies

reactants (gas phase) \rightarrow products (gas phase)

$$\Delta H = \sum \text{enthalpy bonds broken}$$

$$\Delta H > 0 \text{ endothermic}$$

$$\Delta H = \sum \text{enthalpy bonds formed}$$

$$\Delta H < 0 \text{ exothermic}$$

atoms in gas phase

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$\Delta H_{\text{reaction}}$ from bond enthalpies

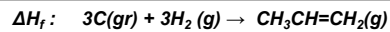
TABLE B.4 Average Bond Enthalpies (kJ/mol)

Single Bonds							
C-H	413	N-H	391	O-H	463	F-F	155
C-C	348	N-N	163	O-O	146		
C-N	293	N-O	201	O-F	190	Cl-F	253
C-O	358	N-F	272	O-Cl	203	Cl-Cl	242
C-F	485	N-Cl	200	O-I	234		
C-Cl	328	N-Br	243	S-H	339	Br-F	237
C-Br	276	H-H	436	S-F	327	Br-Cl	218
C-I	240	H-F	567	S-Cl	253	Br-Br	193
C-S	259	H-Cl	431	S-Br	218	I-Cl	208
Si-H	323	H-Br	366	S-S	266	I-Br	175
Si-S	226	H-I	299	S-Se	266	I-I	151
Si-Cl	301						
Si-O	368						
Multiple Bonds							
C=C	614	N=N	418	O ₂	495		
C≡C	839	N≡N	941				
C=N	615	N=O	607	S=O	523		
C≡N	891			S=Se	418		
C=O	799						
C=O	1072						

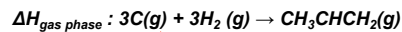
<http://wps.prenhall.com/wps/media/objects/165/169060/tool0801.gif>

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example ΔH_f $\text{CH}_3\text{CH}=\text{CH}_2(\text{g})$

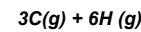


$$3\Delta \bar{H}_{\text{sub}}(\text{C}) = 3(717) \text{ kJ}$$



$$\Delta H = 3\text{BE}(\text{H}_2) = 3(436 \text{ kJ})$$

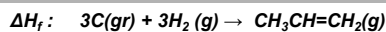
$$\Delta H = -6\text{BE}(\text{C-H}) - \text{BE}(\text{C-C}) - \text{BE}(\text{C=C}) = -6(413 \text{ kJ}) - (348 \text{ kJ}) - (614 \text{ kJ})$$



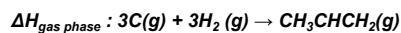
$$\Delta H_f = (3 \times 717 + 3 \times 436 - 6 \times 413 - 348 - 614) \text{ kJ} = 19 \text{ kJ}$$

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example ΔH_f $\text{CH}_3\text{CH}=\text{CH}_2(\text{g})$



$$3\Delta \bar{H}_{\text{sub}}(\text{C}) = 3(717) \text{ kJ}$$



$$\Delta H = 3\text{BE}(\text{H}_2)$$

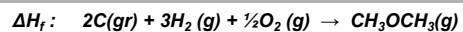
$$\Delta H = -6\text{BE}(\text{C-H}) - \text{BE}(\text{C-C}) - \text{BE}(\text{C=C})$$

TABLE 4.2 THERMODYNAMIC DATA FOR SELECTED ORGANIC COMPOUNDS

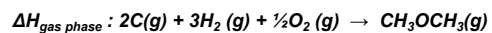
Substance	Formula	Molecular Weight	ΔH_f° (kJ mol ⁻¹)
Propene(g)	C ₃ H ₆	42.08	20.0

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example ΔH_f $\text{CH}_3\text{OCH}_3(\text{g})$



$$2\Delta \bar{H}_{\text{sub}}(\text{C}) = 2(717) \text{ kJ}$$



$$\Delta H = 3\text{BE}(\text{H}_2) + \frac{1}{2}\text{BE}(\text{O}_2) = 3(436 \text{ kJ}) + \frac{1}{2}(495 \text{ kJ})$$

$$\Delta H = -6\text{BE}(\text{C-H}) - 2\text{BE}(\text{C-O}) = -6(413 \text{ kJ}) - 2(358 \text{ kJ})$$



$$\Delta H_f = (2 \times 717 + 3 \times 436 + \frac{1}{2} \times 495 - 6 \times 413 - 2 \times 358) \text{ kJ} = -184.1 \text{ kJ}$$

Substance	Formula	Molecular Weight	ΔH_f° (kJ mol ⁻¹)
Dimethyl ether(g)	C ₂ H ₆ O	131.6	-184.1

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bond enthalpy vs bond energy

- often [mis]used interchangeably
Usually both meant to mean **enthalpy**
- bond **enthalpy**: thermodynamic heat measured at const P
- bond **energy**: the bond strength from quantum mechanical calculation
- can be interconverted by the $\Delta H = \Delta U + \Delta n_{\text{gas}}RT$ relation (p. 68; example problem 4.1 for O-H bond *bond energy* = 461 kJ mol^{-1} vs *bond enthalpy* = $463.5 \text{ kJ mol}^{-1}$)
- Table 4.3 E&R is weird (hard to read)

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table 4.3 E&R

TABLE 4.3 MEAN BOND ENERGIES (kJ/mol)

1 2 Selected Bond Energies (kJ/mol)

3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18

19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100

101 102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119 120 121 122 123 124 125 126 127 128 129 130 131 132 133 134 135 136 137 138 139 140 141 142 143 144 145 146 147 148 149 150 151 152 153 154 155 156 157 158 159 160 161 162 163 164 165 166 167 168 169 170 171 172 173 174 175 176 177 178 179 180 181 182 183 184 185 186 187 188 189 190 191 192 193 194 195 196 197 198 199 200

201 202 203 204 205 206 207 208 209 210 211 212 213 214 215 216 217 218 219 220 221 222 223 224 225 226 227 228 229 230 231 232 233 234 235 236 237 238 239 240 241 242 243 244 245 246 247 248 249 250 251 252 253 254 255 256 257 258 259 260 261 262 263 264 265 266 267 268 269 270 271 272 273 274 275 276 277 278 279 280 281 282 283 284 285 286 287 288 289 290 291 292 293 294 295 296 297 298 299 300

301 302 303 304 305 306 307 308 309 310 311 312 313 314 315 316 317 318 319 320 321 322 323 324 325 326 327 328 329 330 331 332 333 334 335 336 337 338 339 340 341 342 343 344 345 346 347 348 349 350 351 352 353 354 355 356 357 358 359 360 361 362 363 364 365 366 367 368 369 370 371 372 373 374 375 376 377 378 379 380 381 382 383 384 385 386 387 388 389 390 391 392 393 394 395 396 397 398 399 400

401 402 403 404 405 406 407 408 409 410 411 412 413 414 415 416 417 418 419 420 421 422 423 424 425 426 427 428 429 430 431 432 433 434 435 436 437 438 439 440 441 442 443 444 445 446 447 448 449 450 451 452 453 454 455 456 457 458 459 460 461 462 463 464 465 466 467 468 469 470 471 472 473 474 475 476 477 478 479 480 481 482 483 484 485 486 487 488 489 490 491 492 493 494 495 496 497 498 499 500

501 502 503 504 505 506 507 508 509 510 511 512 513 514 515 516 517 518 519 520 521 522 523 524 525 526 527 528 529 530 531 532 533 534 535 536 537 538 539 540 541 542 543 544 545 546 547 548 549 550 551 552 553 554 555 556 557 558 559 560 561 562 563 564 565 566 567 568 569 570 571 572 573 574 575 576 577 578 579 580 581 582 583 584 585 586 587 588 589 590 591 592 593 594 595 596 597 598 599 600

601 602 603 604 605 606 607 608 609 610 611 612 613 614 615 616 617 618 619 620 621 622 623 624 625 626 627 628 629 630 631 632 633 634 635 636 637 638 639 640 641 642 643 644 645 646 647 648 649 650 651 652 653 654 655 656 657 658 659 660 661 662 663 664 665 666 667 668 669 670 671 672 673 674 675 676 677 678 679 680 681 682 683 684 685 686 687 688 689 690 691 692 693 694 695 696 697 698 699 700

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2301 2302 2303 2304 2305 2306 2307 2308 2309 2310 2311 2312 2313 2314 2315 2316 2317 2318 2319 2320 2321 2322 2323 2324 2325 2326 2327 2328 2329 2330 2331 2332 2333 2334 2335 2336 2337 2338 2339 2340 2341 2342 2343 2344 2345 2346 2347 2348 2349 2350 2351 2352 2353 2354 2355 2356 2357 2358 2359 2360 2361 2362 2363 2364 2365 2366 2367 2368 2369 2370 2371 2372 2373 2374 2375 2376 2377 2378 2379 2380 2381 2382 2383 2384 2385 2386 2387 2388 2389 2390 2391 2392 2393 2394 2395 2396 2397 2398 2399 2400

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Chemistry 163B Winter 2013

Lectures 6-7 Thermochemistry

TABLE 4.1 (CONTINUED)

Substance	ΔH_f° (kJ mol ⁻¹)	ΔG_f° (kJ mol ⁻¹)	S° (J mol ⁻¹ K ⁻¹)	$C_{p,m}^\circ$ (J mol ⁻¹ K ⁻¹)	Atomic or Molecular Weight (amu)
H ₂ (g)	218.0	203.3	114.7	20.8	1.008
OH ₂ (g)	39.0	34.2	183.7	29.9	17.01
H ₂ O(g)	-241.8	-228.6	188.8	33.6	18.015
H ₂ O(l)	-285.8	-237.1	70.0	75.3	18.015
H ₂ O(s)			48.0	36.2 (273 K)	18.015
H ₂ O ₂ (g)	-136.3	-105.6	232.7	43.1	34.015
H ⁺ (aq)	0	0	0		1.008
OH ⁻ (aq)	-230.0	-157.24	-10.9		17.01
Carbon					
Graphite(s)	0	0	5.74	8.52	12.011
Diamond(s)	1.89	2.90	2.38	6.12	12.011
C(s)	716.7	671.2	158.1	20.8	12.011
CO(g)	-110.5	-137.2	197.7	29.1	28.011
CO ₂ (g)	-393.5	-394.4	213.8	37.1	44.010
HCN(g)	135.5	124.7	201.8	35.9	27.03
CN ⁻ (aq)	150.6	172.4	94.1		26.02
HCO ₂ ⁻ (aq)	-692.0	-586.8	91.2		61.02
CO ₃ ²⁻ (aq)	-675.2	-527.8	-50.0		60.01
Oxygen					
O ₂ (g)	0	0	205.2	29.4	31.999
O(g)	249.2	231.7	161.1	21.9	15.999
O ₃ (g)	142.7	163.2	238.9	39.2	47.998
OH ₂ (g)	39.0	34.22	183.7	29.9	17.01
OH ⁻ (aq)	-230.0	-157.2	-10.9		17.01

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E&R prob 4.20b HW3 #16

P4.20 If 3.059 g of ethanol, C₂H₅OH(l) is burned completely in a bomb calorimeter at 298.15 K, the heat produced is 90.447 kJ.

- Calculate $\Delta H_{\text{combustion}}^\circ$ for ethanol at 298.15 K.
- Calculate ΔH_f° of ethanol at 298.15 K.

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TABLE 4.1 (CONTINUED)

Substance	ΔH_f° (kJ mol ⁻¹)	ΔG_f° (kJ mol ⁻¹)	S° (J mol ⁻¹ K ⁻¹)	$C_{p,m}^\circ$ (J mol ⁻¹ K ⁻¹)	Atomic or Molecular Weight (amu)
H ₂ (g)	218.0	203.3	114.7	20.8	1.008
OH ₂ (g)	39.0	34.2	183.7	29.9	17.01
H ₂ O(g)	-241.8	-228.6	188.8	33.6	18.015
H ₂ O(l)	-285.8	-237.1	70.0	75.3	18.015
H ₂ O(s)			48.0	36.2 (273 K)	18.015
H ₂ O ₂ (g)	-136.3	-105.6	232.7	43.1	34.015
H ⁺ (aq)	0	0	0		1.008
OH ⁻ (aq)	-230.0	-157.24	-10.9		17.01
Carbon					
Graphite(s)	0	0	5.74	8.52	12.011
Diamond(s)	1.89	2.90	2.38	6.12	12.011
C(s)	716.7	671.2	158.1	20.8	12.011
CO(g)	-110.5	-137.2	197.7	29.1	28.011
CO ₂ (g)	-393.5	-394.4	213.8	37.1	44.010
HCN(g)	135.5	124.7	201.8	35.9	27.03
CN ⁻ (aq)	150.6	172.4	94.1		26.02
HCO ₂ ⁻ (aq)	-692.0	-586.8	91.2		61.02
CO ₃ ²⁻ (aq)	-675.2	-527.8	-50.0		60.01
Oxygen					
O ₂ (g)	0	0	205.2	29.4	31.999
O(g)	249.2	231.7	161.1	21.9	15.999
O ₃ (g)	142.7	163.2	238.9	39.2	47.998
OH ₂ (g)	39.0	34.22	183.7	29.9	17.01
OH ⁻ (aq)	-230.0	-157.2	-10.9		17.01

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TABLE 4.2 THERMODYNAMIC DATA FOR SELECTED ORGANIC COMPOUNDS AT 298.15 K

Substance	Formula	Molecular Weight	ΔH_f° (kJ mol ⁻¹)	$\Delta H_{\text{combustion}}^\circ$ (kJ mol ⁻¹)	ΔG_f° (kJ mol ⁻¹)	S° (J mol ⁻¹ K ⁻¹)	$C_{p,m}^\circ$ (J mol ⁻¹ K ⁻¹)
Carbon (graphite)	C	12.011	0	-393.5	0	5.74	8.52
Carbon (diamond)	C	12.011	1.89	-395.4	2.90	2.38	6.12
Carbon monoxide	CO	28.01	-110.5	-283.0	-137.2	197.7	29.1
Acetone(l)	C ₃ H ₆ O	58.08	-248.4	-1790	-155.2	199.8	126.3
Benzene(l)	C ₆ H ₆	78.12	49.1	-3208	124.5	173.4	136.0
Benzene(g)	C ₆ H ₆	78.12	97.9	-3303	129.7	269.2	82.4
Benzoic acid(s)	C ₇ H ₆ O ₂	122.13	-385.2	-3227	-245.5	167.6	146.8
1,3-Butadiene(g)	C ₄ H ₆	54.09	110.0	-2541			79.8
Dimethyl ether(g)	C ₂ H ₆ O	46.07	-184.1	-1480	-112.6	266.4	64.4
Ethanol(g)	C ₂ H ₆ O	46.07	-84.0	-1361	-32.0	229.2	52.5
Ethanol(l)	C ₂ H ₆ O	46.07	-277.6	-1367	-174.8	160.7	112.3
Ethanol(s)	C ₂ H ₆ O	46.07	-234.8	-1367	-167.9	281.6	65.6
Ethene(g)	C ₂ H ₄	28.05	52.4	-1411	68.4	219.3	42.9
Ethyne(g)	C ₂ H ₂	26.04	227.4	-1310	209.2	200.9	44
Formaldehyde(g)	CH ₂ O	30.03	-108.6	-571	-102.5	218.8	35.4

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standard states and standard heats of formation

standard state (°): gas partial pressure 1 bar
 liquid or solid pure substance at 1 bar
 solute in soln 1 M

standard molar heat of formation (H_f°):
 $(\Delta H_T^\circ)_{\text{reaction}}$ where 1 mole of substance is produced
 from **elements in their most stable form at given temperature**

\bar{H}_f° at 298K in kJ/mol

C(gr)=0 O₂(g)=0 C(dia)=1.89 H₂O(g)=-241.8 H₂O(l)=-285.8
 F₂(g)=0 Cl₂(g)=0 I₂(g)=62.4 I₂(s)=0

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