DERIVE ΔG EQUATION FOR CHEMICAL WORK

Cell Biology 3611

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There is too much detail here for you to memorize for an exam; however I expect the better student to read through this and make a real attempt at understanding the steps. You will get an understanding of

- **how mathematics is used by a biologist,**
- **why you take mathematics courses even though you are a biology major**
- **limitations or assumptions of the ΔG equation that are not emphasized in chemistry classes. That is, biologists emphasize electrical work and this form of the Gibb's equation totally ignores this crucial type of work.**
- **Note that we will talk in a later chapter (ch. 8) in our text (World of the Cell by Becker et al.) about how you would modify this equation to include electrical work.**
- **the textbook material --Chapter 5- see the textbook's version of this derivation.**

So, don't memorize the derivation but understand it—ESP IMPORTANT: know the assumptions.
I might ask you an extra credit question on the exam, but I will not ask you detailed questions on this derivation on the exam (but know how to use the 2 final equations as we discussed in lecture). However, understanding the equation will help you use the equations on exams; even simply reading this thoroughly will help you with the equations – a good way of studying!!

SEE **TEXT section entitled: BIOENERGETICS in chapter 5. See EQUATIONS IN TEXT BOOK (World of the Cell by Becker et al.) 5-1 TO the end of chapter.**
I have attempted to PROVIDE MORE EXPLANATION FOR THESE EQUATIONS BELOW.

DEFINE (follow along in text): SYSTEM VS. SURROUNDINGS.

Since ENERGY IS NOT CREATED OR DESTROYED:

EQUATION (1) $\Delta E = Q - W$

WHERE **ΔE** IS THE CHANGE (Δ MEANS "CHANGE" OR (LAST STATE)-(ORIGINAL STATE)) IN **INTERNAL ENERGY of a system (could be the cell or an organelle)**,

Q IS HEAT LOST TO THE SYSTEM.

"**W" IS THE WORK THAT THE SYSTEM DOES ON THE SURROUNDINGS**. WORK MAY BE TO MAKE A PROTEIN, MAKE ATP, MOVE AN ION ACROSS A MEMBRANE, CAUSE A CELL TO SWELL, CHANGE THE SHAPE OF A PROTEIN. WORK WILL FALL INTO THE CATEGORIES THAT WE DESCRIBED:

MECHANICAL, ELECTRICAL, AND CHEMICAL (and heat but we will not emphasize this type). NOTE WORK ON THE SURROUNDINGS HAS A **NEGATIVE** SIGN (some derivations have opposite sign, +, for same idea).

FIRST, WE WILL LOOK **ONLY AT CHEMICAL WORK** AND DERIVE THE GIBB'S FREE ENERGY EQUATION.
FOR ALL OF OUR EQUATIONS: YOU WILL NOT HAVE TO REGURGITATE THE DERIVATION BUT MUST UNDERSTAND THE ASSUMPTIONS INVOLVED IN THE DERIVATION.

LATER (chapt. 8), WE WILL LOOK AT THE COMBINATION OF **CHEMICAL AND ELECTRICAL WORK**--THIS IS THE COMBINATION THAT THE CELL BIOLOGIST MOST COMMONLY USES.

(2) Q IS EQUAL TO TEMPERATURE MULTIPLIED BY ENTROPY (ENTROPY IS HOW RANDOM OR SCATTERED THE SYSTEM IS, VERSUS HOW ORGANIZED IT IS) –THIS IS **Δ(TS).**
WORK IS OF THE TYPES NOTED ABOVE. NOW LETS SUBSTITUTE IN FOR Q AND FOR WORK TERMS:

ΔE = Δ(TS) - Δ(MECH. WORK + ELEC. WORK + CHEMICAL WORK)

= Δ(TS) - Δ(PV + ZV + μN)

NOTE MECHANICAL WORK IS PV (PRESSURE* VOLUME), ELECTRICAL WORK IS ZV (CHARGE OF ION*VOLTAGE), AND CHEMICAL WORK IS μN (CHEMICL POTENTIAL* NUMBER OF MOLECULES INVOLVED).

(3) **FIRST ASSUMPTION:** CHEMISTS TYPICALLY ASSUME **THAT ALL WORK IS CHEMICAL WORK ONLY** (NO ELECTRICAL OR MECHANICAL; SOMETIMES THERE IS NO CHANGE IN PRESSURE OR VOLUME AS CHEMICAL REACTION TAKES PLACE SO THERE IS NO MECHANICAL WORK. OFTEN, NO ELECTRICAL WORK IS DONE AS NO ION MOVES IN ELECTRICAL FIELD).

THUS WE CAN THEN DEFINE **ΔH** IS THE CHANGE IN ENTHALPY OF A CHEMICAL REACTION. THIS IS THE **CHANGE IN ENTHALPY- CHANGE IN CHEMICAL BONDS.**

ΔH = (ENERGY REQUIRED TO BREAK BONDS) - (ENERGY GIVEN OFF BY NEW BOND FORMATION)
AS WE ASSUMED NO OTHER FORM OF WORK IS DONE (NO MECHANICAL, ELECTRICAL), THIS IS THE ONLY TYPE OF CHANGE OF ENERGY WITHIN THE SYSTEM (INTERNAL ENERGY). SO WE CAN SET :

ΔH = ΔE THAT IS, THE CHANGE IN CHEMICAL BONDS IS THE ONLY FORM OF INTERNAL ENERGY CHANGE IN THE SYSTEM (NO ENERGY GOES TO MECHANICAL/ELECTRICAL WORK). This is the result of assumption one.

THE SECOND ASSUMPTION: TEMPERATURE IS CONSTANT (ALTHOUGH NOT TRUE FOR MOST PLANTS AND ANIMALS, OUR BODY IS AT CONSTANT TEMP; WE CAN IGNORE $S\Delta T$ SINCE IT IS = 0; ΔT IS ZERO):

(4) SUBSTITUTE FOR ΔE IN EQUATION (2) AND GET RID OF ELECTRICAL AND MECHANICAL WORK TERMS:

$\Delta H = T\,\Delta S - \Delta(\mu N)$
(EXPLAIN THE LAST TERM….CHANGE IN CHEMICAL WORK)

(5) REARRANGE AND RENAME:
ΔG= GIBB'S FREE ENERGY CHANGE = $- \Delta\mu N = \Delta H - T\Delta S$

SO GIBB'S FREE ENERGY CHANGE IS ONLY GOOD FOR CHEMICAL WORK BUT WILL NOT BE ACCURATE FOR PROCESSES INVOLVING MECHANICAL OR ELECTRICAL WORK.

IN YOUR OWN WORDS, SUMMARIZE 2 ASSUMPTIONS OF THE GIBB'S EQUATION BELOW:

HOWEVER, THIS FORM OF THE ΔG EQUATION **IS NOT USED BY CELL BIOLOGISTS** (YOU CANT EASILY MEASURE THE CHANGE IN ENTROPY ΔS). SO, WE HAVE TO CHANGE THE EQUATION TO A FORM THAT CAN ACTUALLY BE USED:

(6) FROM EQUATION (5), NOTE THAT
$\Delta G = -\Delta(\mu N)$

AND THAT THE CHANGE IN CHEMICAL POTENTIAL* NUMBER OF MOLECULES IS THE CHANGE IN ONE MULTIPLIED BY THECHANGE IN THE SECOND (IF YOU HAVE HAD CALCULUS, THIS MAKES MORE SENSE):

$-\Delta(\mu N) = -(\mu\,\Delta N + N\,\Delta\mu)$

HOWEVER, THERE IS NO CHANGE IN THE NUMBER OF MOLECULES SO "ΔN" IS ZERO AND THIS TERM ($\mu\Delta N$) DROPS OUT; LEAVING

(7) **$\Delta G = N\,\Delta\mu$**

(8) AND N =1 (ONE MOLE) SO **$\Delta G = \Delta\mu$**

(9) **DEFINE μ = CHEMICAL POTENTIAL** =
$\mu = \mu_O + RT\ Ln\ (CONC)$
NOTE USE OF NATURAL LOG (Ln). "R" IS 1.98 CAL/(MOL-DEG.K). "T" IS DEG.

KELVIN (CENTIGRADE + 273). **μ_O IS THE CHEMICAL POTENTIAL UNDER STANDARD CONDITIONS, AND THE RTLn TERM IS A CORRECTION FACTOR.**

(10) REMEMBER THE CHANGE IN GIBB'S FREE ENERGY IS THE DIFFERENCE BETWEEN REACTANTS AND PRODUCTS:

$\Delta G = \Delta\mu = \mu_{PRODUCTS} - \mu_{REACTANTS}$

FOR EXAMPLE: FOR A REACTION SUCH AS A + B --> C + D

$$\Delta\mu = \mu_C + \mu_D - \mu_A + \mu_B$$

(11) $\Delta G = (\mu_O + RT\ Ln(PROD)) - (\mu_O + RT\ Ln(REACT))$

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(12) REARRANGING AND USING THIS SIMPLE RULE FROM MATHEMATICS: LnB -LnA = Ln (B/A) TO CHANGE TO THE FORM IN (12) BELOW.

WE GET TO A FORM THAT WE CAN USE:

$\Delta G' = \Delta G_O' + RT\ Ln\ ([PRODUCTS]/\ [REACTANTS])$

(SEE TEXTBOOK EQUATIONS 5-16 THROUGH 5-23)

(IF YOU WANT TO, YOU CAN SWITCH OVER TO LOG BASE 10 SINCE: 2.303 LOG X = LnX)

NOTE THAT **$\Delta G_O'$ REFERS TO STANDARD CONDITIONS** (PH 7, 1 ATM, TEMP 25C, CONC. 1 MOLAR).

*****REMEMBER THAT THIS IS FOR A < == > B; WHAT IF 2A < == > B? USE $[A]^2$.**

NOTE THAT CELLS ARE NEVER UNDER STANDARD CONDITIONS—THIS **$\Delta G_O'$ IS SOMETHING THAT WE PICK UP FROM A TABLE OR CALCULATE USING Keq.**
THE SECOND TERM (RT ETC.) IS THE CORRECTION FOR ACTUAL CELLULAR CONDITIONS SINCE THEY DIFFER FROM STANDARD CONDITIONS.

(13) **EXAMPLES:** AT EQUILIBRIUM, FORCES ACTING UPON THE SYSTEM ARE BALANCED, THUS, NO CHANGE IS TAKING PLACE. WHAT IS $\Delta G'$ AT EQUILIBRIUM? (ANSWER: $\Delta G' = 0$ AT EQUILIBRIUM)

FOR EXAMPLE, THE REACTION A <--> B. IF A GOES TO B (A NET FORWARD REACTION) THEN THE SYSTEM IS NOT IN EQUILIBRIUM. AT EQUILIBRIUM, IF A LITTLE B GOES TO A, A LITTLE A GOES TO B-THUS, THERE IS NO NET CHANGE IN CONCENTRATIONS.

CAN ANY CHEMICAL WORK BE DONE AT EQUILIBRIUM??? NO; YOU'RE DEAD.