


## Entropy vs enthalpy driven

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At the beginning of the year, I wrote about the use of calorimetry in drug detection. Years ago, these people would have raised eyebrows if they had suggested it, but it is becoming more popular, especially among people who discover shingles-based drugs. After all, the binding energy we rely on for our drug candidates is a thermodynamic trait, and you can detect heat that drifts away when molecules bond well. Calorimetry also allows you to break down its energy binding down to its enthalpy (delta-H) and entropy (T delta-S) components, which is difficult to do by other means. And that's where the fight starts. As I mentioned back in March, one of the ideas that has hovered around is that better drug molecules have a more enhanced contribution to their binding. Roughly, enthalpic interactions are often what inter-chemists call positive as the formation of new hydrogen bonds or pi-stack, and entropy interactions are often only due to pushing water molecules with proteins with some oily part of your molecule. (Note: There are several complex exceptions for double-rounding from both of these mental models. Thermodynamics is an ingenious field!) In this way, it makes sense that more robust compounds with better properties may be more enhanced in their binding. But we don't live in a world that is being mesmed by what makes intuitive sense. Some people think that the examples cited in the literature for this effect are the only decent examples anyone has. At a conference on fragments I attended last week, however, a speaker from Astex (a company that certainly runs a lot of project optimization fragments) said that they basically do not see it. In their hands are some series of enthalpy-driven pencils as they get better, some entropy drive, and some gear switches as SAR develops. Another speaker said they are on the other side to go with enthalpy-driven compounds, but I'm not sure if that's just because they don't have as much data as astex people have. As far as I'm concerned, the whole concept I talked about in March is still in an interesting but undokakana category. We're all looking for new ways to pick better initial compounds or optimize leads, but I'm still not sure if this will do the trick. . Gibbs' energy is the energy of a chemical reaction that can be used for non-mechanical work. Gibbs Energy is described as  $G = H - TS$  Where H is enthalpy, the T is the temperature and S is entropy.  $\Delta G$  is used to predict spontaneity within the system with  $\Delta G_{sys} = \Delta H_{sys} - T\Delta S_{sys}$  Gibbs energy was developed in the 1870s by Josiah Willard Gibbs. He initially thought of this energy as the energy available in the system. His article was published in 1873, Graphic Methods in the equation can predict the behavior of systems when they are combined. At constant temperature and pressure, the Gibbs system energy can be described as  $\Delta G_{sys} = \Delta H_{sys} - T\Delta S_{sys}$  This equation can be used to determine the spontaneity of the process. If  $\Delta G_{sys} \leq 0$ , the process is spontaneous. If  $\Delta G_{sys} = 0$ , the system is in balance. If  $\Delta G_{sys} > 0$ , the procedure is not spontaneous. If  $\Delta G_{sys} < 0$ , the procedure is exergonic. If  $\Delta G_{sys} > 0$ , the procedure is endergonic. Gibbs Energy is a useful tool for describing how the response is conducted. If  $\Delta H > 0$ , the reaction is enthalpic. However, if  $\Delta S > 0$ , the reaction is entropic. Clausius-Clapeyronova enačba je aplikacija, ki izhaja iz Gibbova energija:  $\ln \left( \frac{P_2}{P_1} \right) = \frac{\Delta H_{vap}}{R} \left( \frac{1}{T_1} - \frac{1}{T_2} \right)$  Druga pomembna aplikacija Gibb-ove energije je Maxwellova relacija (dostopna i na linku na koncu wiki strani.) Če tak & amp; temperatura reakcije ni konstanta,  $\left( \frac{\partial G}{\partial T} \right)_P = -S$  Za infinitesimalen proces,  $\Delta G = \Delta H - T\Delta S$  Za reakcijo, kjer je temperatura stalna,  $\Delta G = \Delta H - T\Delta S$  Iz Prvega zakona termodinamike, mi vemo  $\Delta H = U + PV$  We find that  $\Delta G = \Delta H - T\Delta S$  showing the obvious dependence of  $\Delta G$  on temperature and pressure. To observe the change Gibbs energy due to the change in temperature itself (pressure constant) equation becomes  $\Delta G = -S\Delta T$  Rescue for S and connection to Eq. (1) The Gibbs-Helmholtz equation is found:  $\left( \frac{\partial (\Delta G/T)}{\partial T} \right)_P = -\frac{\Delta H}{T^2}$  Gibbs-Helmholtz equation is very important, in order to change Gibbs's energy to her temperature dependency, i position balance to change u enthalpy. To observe the change Gibbs energy due to a change in pressure itself (temperature holds constant) the equation becomes  $\Delta G = V\Delta P$  If it is assumed that the gas is ideal then  $\Delta G = nRT \ln \left( \frac{P_2}{P_1} \right)$  for initial i-ending pressure (P1 i P2) at constant T. Gibbs Energy is defined as a status function (to your ownity, which depends only on the state describing the system, not how to change the stasis function.) This is because each component of the equation (H, T and S) is all state functions. That's why we can know about Gibbs' power change without knowing all the details of the process. In a process that takes place at constant temperature and pressure (298 K, 1 atm), the standard molar free energy formation can be determined by changing the free from reactors and products. Use predefined values, Eqn. (17) Can be used  $\Delta G^\circ = \sum G^\circ_{products} - \sum G^\circ_{reactants}$  Standard-State Free Energy Reactions Gibbs Energy the standard state is applied to the standard state using  $\Delta G^\circ = \Delta H^\circ - T\Delta S^\circ$   $\Delta H^\circ$  i  $\Delta S^\circ$  values shall be applied to the addition of the chemistry textbook, nor the use of this link. Gibbs energy can be found in all conditions by indicating the energy of the reaction without a standard state using  $\Delta G = \Delta G^\circ + RT \ln Q$  Where Q is the corner of the reaction. Very rarely does chemistry actually occur under the terms of the standard state. Using the above equation and the standard state values, the chemists can determine the entire gibb-th energy for the system, regardless of the conditions. References Olmsted, J. Chemistry, 4. John Wiley & Sons, Inc.: Hoboken 2006. Chang, R. Physical Chemistry for Biosciences; University Science Books: Sausalito, 2005. Christian, S.D. Gibbs-Duhem equation and free energy calculations. J. Chem. Educ. 1962, 39 (10) 521-524. Porter, S.K. Volume-entropy-energy surface J.W. Gibbs. J. Chem Educ. 1971, 48(4) 231-234. Problems Calculate the energy of formations without the standard state for H2O2(l) from H2 and O2 according to the following values:  $\Delta G_f^\circ(\text{H}_2\text{O}_2)$ : 0 kJ/mol  $\Delta G_f^\circ(\text{O}_2)$ : 0 kJ/mol  $\Delta G_f^\circ(\text{H}_2\text{O}_2)$ : -120.4 kJ/mol Natuk: (product\*coefficient) - [(Reaktant1\*coefficient)+(Reaktans2\*coefficient)] Consider the reaction trail:  $\text{CaCO}_3 \rightarrow \text{CaO} + \text{CO}_2$  At how much temperature would this reaction become favourable? Note: Assume that  $\Delta H^\circ$  and  $\Delta S^\circ$  are temperature independent. Values: Substance  $\Delta H^\circ_f$   $\text{CaCO}_3$  -1206.9 kJ/mol 92.9 J/K mol  $\text{CaO}$  -635.6 kJ/mol 39.8 J/K mol  $\text{CO}_2$  -393.5 kJ/mol 213.6 J/K mol Natuk: How much of the value  $\Delta G$  the reaction becomes spontaneous, i therefore favorable? Then look for the  $\Delta H$  value for the reaction (product-reaktivants) and the  $\Delta S$  value for the reaction (reactantani-products.) Save for T. Is the above decomposition calcium carbonate enthalpy drive or entropy drive? Tip: Is  $\Delta H > 0$ ,  $\Delta S > 0$ ,  $\Delta H > 0$ ,  $\Delta S > 0$ ? Tip: 120.4 kJ/mole 1107.8 K Enthalpy Interlocutor Christine Gobrogge (Hope College) Chapter 14: Department of Thermodynamics 14-1: Declaration of sign of change of entropy, section  $\Delta S$  14-2: Calculation  $\Delta S^\circ$  Using standard entropy,  $S^\circ$  Section 14-3: Second Law of Thermodynamics | Gibbs free energy change,  $\Delta G$  Section 14-4: The Effect of Temperature on  $\Delta G$  and the Spontaneity of Reactions Section 14-5: Calculating  $\Delta G^\circ$  from Standard Gibbs Free Energies of Formation,  $\Delta G^\circ_f$  Chapter 14 Practice exercises i review Quizzes Section 14-1: Predict the sign of entropic change,  $\Delta S$ , but thermochemisia is primarily focused on heat, grounded u chemical reactions, thermodynamics explores the role of energy General. Entropy (S) is essentially an indicator of the level of disruption or chaos in a given system. The following processes usually occur with an increase in entropy and thus a positive change in entropy ( $\Delta S$ ): 1. The temperature of the substance is increased. 2. The solid is converted into liquid, solution or gas (sublimation). 3. The liquid is converted into gas. 4. Chemical reaction in which the number of gas moles increases (the sum of the gas coefficients between the products on the right side is greater than the sum of the coefficients of gas between the reactants on the left). If the number of gas moles does not change during a chemical reaction, more information is generally needed to determine the  $\Delta S$  sign. The following processes usually occur with a reduction in entropy and thus negative  $\Delta S$ : 1. The temperature of the substance is reduced. 2. The solid is formed from a liquid, solution or gas. 3. The gas is converted into liquid. 4. Chemical reaction in which the number of gas moles decreases. Sample exercise 14A: Predicts the  $\Delta S$  sign for each process: (a) The water cools from 35 °C to 25 °C. (b) Liquid ethanol freezes. (c) Solid iodine is dissolved in carbon disulphide. (d) 3 S (s) + 2 H2O (g) → SO2 (g) + 2 H2S (g) (e) Niium fumes. (f) CO (g) + H2O (g) → CO2 (g) + H2 (g) (g) Solution: (a) Temperature is reduced, so that  $\Delta S < 0$ . (b) Liquid to solid so that  $\Delta S < 0$ . (c) Solid to solution so that  $\Delta S > 0$ . (d) Although the total mole is reduced (3 + 2 → 1 + 2), the moles of the gas are increased (2 → 1 + 2). Therefore,  $\Delta S > 0$ . (e) Gas → the liquid, so that  $\Delta S < 0$ . (f) Gas moles are unchanged (1 + 1 → 1 + 1), so more information is needed to determine the  $\Delta S$  sign. Section 14-2: Calculation  $\Delta S^\circ$  Using standard entropies,  $S^\circ$  We can calculate the standard entropy change,  $\Delta S^\circ$ , for reaction u unit J/mol·To use standard product entropys as follows: Sample Exercise 14B: Predict the  $\Delta S^\circ$  sign, then calculate the value  $\Delta S^\circ$  for reaction N2 (g) + 3 F2 (g) → and 2 NF3 (g) using the following information Substance  $S^\circ$  (J/mol·K) F2 (g) 203 N2 (g) 192 NF3 (g) 261 Solution:  $\Delta S^\circ$  is ocekiva to be negative, so 100 moles are gased by the snail u reaction (1 + 3 → 2).  $\Delta S^\circ = [2(261) - 1(192) - 3(203)] \text{ J/mol}\cdot\text{K} = -279 \text{ J/mol}\cdot\text{K}$  Section 14-3: Second Law of Thermodynamics and Gibbs Free Energy Change,  $\Delta G$  A spontaneous process is one that will continue to progress without external intervention. Under the second law of thermodynamics, the entropy of the universe must increase as a result of a spontaneous process, and therefore the entropy of the universe must be positive as a result of a spontaneous process. For a chemical reaction, an entropy change in the universe can be considered as the sum of an entropic reaction change and a change of environment involving everything except reaction particles. Therefore, the second law of thermodynamics may be expressed for chemical reactions as follows: spontaneous reaction:  $\Delta S_{universe} = \Delta S_{rxn} + \Delta S_{surroundings}$  &gt; 0  $\Delta S_{surroundings}$  is associated with  $\Delta H_{rxn}$  i Kelvin temperature as follows:  $\Delta S_{surroundings} = -\Delta H_{rxn}/T$ . If  $\Delta S_{surrounding}$  is replaced in the above equation, we get: spontaneous reaction:  $\Delta S_{rxn} - \Delta H_{rxn}/T$  &gt; 0 If both sides of the equation are defined by (T), we get: spontaneous reaction:  $\Delta H_{rxn} - T\Delta S_{rxn}$  &gt; 0 Quantity  $\Delta H_{rxn} - T\Delta S_{rxn}$  is known as Gibbs free energy (or Gibbs energy change),  $\Delta G_{rxn}$ . Therefore,  $\Delta G_{rxn}$  will be negative for spontaneous reaction: spontaneous reaction:  $\Delta G_{rxn} = \Delta H_{rxn} - T\Delta S_{rxn}$  &lt; 0 Note that if  $\Delta G_{rxn}$  and  $\Delta H_{rxn}$  are expressed in kJ/mol,  $\Delta S_{rxn}$  must be first converted from J/mol·K u kJ/mol·K before using that equation. Sample Exercise 14C: For a positive reaction at 75 °C,  $\Delta H = 118 \text{ kJ/mol}$  i  $\Delta S = 175 \text{ J/mol}\cdot\text{K}$ . Calculate  $\Delta G$  for reaction at 75 °C i delay that the reaction is spontaneous at this temperature. Solution: From  $\Delta G$  &gt; 0, the reaction is unpotane at 75 °C. Section 14-4: Effect of temperature on  $\Delta G$  and spontaneousness of reactions Given that the sign temperature Kelvin cannot be negative, we see mathematically that: 1. Reaction with  $\Delta H < 0$  and  $\Delta S > 0$  will have  $\Delta G = \Delta H - T\Delta S$  &lt; 0 at all temperatures. Therefore, the reaction e be spontaneous at all temperatures. How i negative sign  $\Delta H$  i positive sign  $\Delta S$  water to reaction be favorable, reaction is i enthalpy i entropy driven. 2. Reaction with  $\Delta H > 0$  i  $\Delta S > 0$  imat  $\Delta G = \Delta H - T\Delta S$  &gt; 0 at all temperatures. Therefore, the reaction will be unspontane at all temperatures. 3. The reaction with  $\Delta H > 0$  and  $\Delta S > 0$  will have  $\Delta G = \Delta H - T\Delta S$  &lt; 0 only at relatively high temperatures. Therefore, the reaction will only be spontaneous at relatively high temperatures. Since only a positive sign  $\Delta S$  (but not a positive sign  $\Delta H$ ) leads to the benefit of the reaction, the reaction promotes entropy. 4. The reaction with  $\Delta H < 0$  and  $\Delta S < 0$  will have  $\Delta G = \Delta H - T\Delta S$  &lt; 0 only at relatively low temperatures. Therefore, the reaction will only be spontaneous at relatively low temperatures. Since only the negative sign  $\Delta H$  (but not the negative sign  $\Delta S$ ) leads to the benefit of the reaction, the reaction is positive. The above debate is summarised in the following table:  $\Delta H$   $\Delta S$   $\Delta G = \Delta H - T\Delta S$  Reaction is (+) (+) on all T spontaneous at all T, i enthalpy i entropy driven (+) (+) at all T nonspontane at all T, i enthalpy i entropy driven (+) (+) at high T only spontaneously at high T only, entropy driven (-) (-) at low T only spontaneous at low T only, Driven Sample Exercise 14D: determine whether reactions with the following values  $\Delta H$  and  $\Delta S$  will be spontaneous at all temperatures, unspontaneed at all temperatures spontaneous only at high temperatures, or only at low temperatures. Also indicate the driving force for each spontaneous reaction: (a)  $\Delta H = 42 \text{ kJ/mol}$ ,  $\Delta S = 86 \text{ J/mol}\cdot\text{K}$  (b)  $\Delta H = -242 \text{ kJ/mol}$ ,  $\Delta S = 357 \text{ J/mol}\cdot\text{K}$  (c)  $\Delta H = -124 \text{ kJ/mol}$ ,  $\Delta S = -289 \text{ J/mol}\cdot\text{K}$  (d)  $\Delta H = 26 \text{ kJ/mol}$ ,  $\Delta S = -33 \text{ J/mol}\cdot\text{K}$  Solution: (a) spontaneously on high T only, Entropy inductive (b) spontaneous in general T, i entalpiu i entropy drive (c) spontaneously on the nisko T only, enthalpy driven (d) unspontaneously on the i For reactions that are neither spontaneous at all temperatures Nor unspontaneed at all temperatures, mi u equation  $\Delta G = \Delta H - T\Delta S$ , for example, change the reaction from spontaneous to non-spontaneous so that  $\Delta G$  is given to nulu u equation  $\Delta G = \Delta H - T\Delta S$ , but then solved by temperature. Note that the calculated cut-off temperature is only an estimate, since the  $\Delta H$  and  $\Delta S$  values used in the calculation may change significantly as the reaction temperature increases or decreases. Sample exercise 14E: For a reaction with  $\Delta H = -77.1 \text{ kJ/mol}$  and  $\Delta S = -121 \text{ J/mol}\cdot\text{K}$  estimate the circuit breaker temperature in °C, where the reaction varies from spontaneous to non-spontaneous, and also determine whether the reaction is spontaneous above or below this disconnection temperature. Solution: Therefore, the cutting temperature in °C is 637 K - 273 = 364°C. Since both  $\Delta H$  and  $\Delta S$  are negative, the reaction will only be spontaneous below 364 °C. Section 14-5: Calculation  $\Delta G^\circ$  of Standard Gibbs Free Energies of Formation,  $\Delta G^\circ_f$  We can calculate the standard Gibbs free energy change,  $\Delta G^\circ$ , for the reaction directly using standard Gibbs free energies formation of reactanc and products as follows: Note that  $\Delta G^\circ_f = 0$  kJ/mol for all elements in their standard stocks. Sample exercise 14F: Calculate  $\Delta G^\circ$  for reaction 2 H2S (g) + 3 O2 (g) → 2 H2O (l) + 2 SO2 (g) at 25 °C using Sledce information:  $\Delta G^\circ_f$  junction (kJ/mol) at 25 °C H2S (g) -33.6 H2O (l) -237.1 SO2 (g) -300.2 Solution :  $\Delta G^\circ = 0 \text{ kJ/mol}$  for the standard state element O2 (g), so  $\Delta G^\circ = [2(-237.2) + 2(-300.2) - 2(-33.6) - 3(0)] \text{ kJ/mol} = -1007.4 \text{ kJ/mol}$  Hold at the in-doe that  $\Delta G^\circ$  values are calculated using this method of vade only at the temperature indicated by  $\Delta G^\circ_f$  data. At other temperatures,  $\Delta G^\circ$  can be estimated using the equation  $\Delta G^\circ = \Delta H^\circ - T\Delta S^\circ$ . Chapter 14 Exercises and review Quizzes: 14-1) Provides the  $\Delta S$  sign for each process. (a) The ice is melting. (b) 2 C8H18 (l) + 25 O2 (g) → 16 CO2 (g) + 18 H2O (l) (c) The helium gas is heated from room temperature to 200 °C. (d) Dry ice (solid carbon dioxide) sublimi. (e) Sodium chloride crystallises from a saline water solution. (f) liquid methanol 14-1) (a) Solid to liquid so that  $\Delta S > 0$ . (b) Although the total moles increase (2 + 25 → 16 + 18), the moles of the gas are reduced (25 → 16). Therefore  $\Delta S < 0$ . (c) Temperature increase so that  $\Delta S > 0$ . (d) Solid to gas so that  $\Delta S > 0$ . (e) Solid solution so that  $\Delta S > 0$ . (f) Liquid to gas, Thus  $\Delta S > 0$ ; 0.14-2) Predicts the  $\Delta S^\circ$  i sign then calculate the value  $\Delta S^\circ$  for reaction CH4 (g) + 2 O2 (g) → CO2 (g) + 2 H2O (g) use traces information: Substance  $S^\circ$  (J/mol·K) CH4 (g) 186.2 CO2 (g) 213.6 H2O (g) 188.7 O2 (g) 205.0 14-2) The  $\Delta S^\circ$  sign is difficult to predict i be close to zero, so one hundred moles of gas are not replaced (1 + 2 → 1 + 2).  $\Delta S^\circ = [1(213.6) + 2(188.7) - 1(186.2) - 2(205.0)] \text{ J/mol}\cdot\text{K} = -5.2 \text{ J/mol}\cdot\text{K}$  14-3) For a specific reaction at 115 °C,  $\Delta H = -88 \text{ kJ/mol}$  i  $\Delta S = -170. \text{ J/mol}\cdot\text{K}$ . Calculate  $\Delta G$  for a reaction at 115 °C and determine whether the reaction is spontaneous at this temperature. 14-3) From  $\Delta G$  &lt; 0, the reaction is spontaneous at 115 °C. 14-4) Determine whether reactions with the following values  $\Delta H$  and  $\Delta S$  will be spontaneous at all temperatures, unspontaneed at all temperatures, spontaneous only at high temperatures or only spontaneous at low temperatures. Also indicate the driving force for each spontaneous reaction: (a)  $\Delta H = 609 \text{ kJ/mol}$ ,  $\Delta S = -322 \text{ J/mol}\cdot\text{K}$  (b)  $\Delta H = -92 \text{ kJ/mol}$ ,  $\Delta S = -46 \text{ J/mol}\cdot\text{K}$  (c)  $\Delta H = 65 \text{ kJ/mol}$ ,  $\Delta S = 73 \text{ J/mol}\cdot\text{K}$  (d)  $\Delta H = -402 \text{ kJ/mol}$ ,  $\Delta S = 149 \text{ J/mol}\cdot\text{K}$  14-4) (a) non-nented on T (b) spontaneously only on the Nian T, enthalpy driven (c) spontaneously on high T only, entropy pogonio (d) spontaneously on was T, i enthalpy i entropy driven 14-5) For reaction with  $\Delta H = 47.3 \text{ kJ/mol}$  i  $\Delta S = 120. \text{ J/mol}\cdot\text{K}$ , assess the circuit breaker temperature in °C at which the reaction changes from spontaneous to non-spontaneous, and also determine whether the reaction is spontaneous above or below this disconnection temperature. 14-5) Therefore, the disconnection temperature in °C is 394 K - 273 = 121 °C. Since both  $\Delta H$  and  $\Delta S$  are positive, the reaction will only be spontaneous above 121 °C. 14-6) Calculate  $\Delta G^\circ$  for reaction  $\text{Fe}_3\text{O}_4 (\text{s}) + 4\text{H}_2 (\text{g}) \rightarrow 3 \text{Fe} (\text{s}) + 4 \text{H}_2\text{O} (\text{g})$  0 2 Using traces information: Compound  $\Delta G^\circ_f$  (kJ/mol) at 25 °C  $\text{Fe}_3\text{O}_4 (\text{s})$  -1015  $\text{H}_2\text{O} (\text{g})$  -22 22 9 14-6)  $\Delta G^\circ_f = 0 \text{ kJ/mole}$  for standard H2 (g) i Fe (s) status elements, so  $\Delta G^\circ = [3(0) + 4(-229) - 1(-1015) - 4(0)] \text{ kJ/mol} = 99 \text{ kJ/mol}$  Click to review quiz 1 Click to review the quiz 1 Answers

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