Chemistry Lecture #103: Gibbs Free Energy

We can predict if a chemical reaction will occur spontaneously by looking at the ΔH and ΔS of a reaction.

ΔH = -,spontaneous ΔH = +, non-spontaneous
ΔS = +, spontaneous ΔS = -, non-spontaneous.

If a reaction has ΔH = - and ΔS = +, the reaction will be spontaneous. This is a reaction where energy is released and the products are more random than the reactants, making a reaction highly likely.

If a reaction has ΔH = + and ΔS = -, the reaction will not be spontaneous. This is a reaction where energy must be added, and the products will have greater order than the reactants. This type of reaction will not occur spontaneously.

But what if a reaction releases energy, which favors spontaneity, and decreases randomness, which opposes spontaneity? Or, what if a reaction absorbs energy, which opposes spontaneity, but increases randomness, which favors spontaneity?

In circumstances where ΔH and ΔS oppose each other's influence on spontaneity, we can use the Gibbs free energy formula to calculate the spontaneity of a reaction.

$\Delta G = \Delta H - T\Delta S$

ΔG = change in Gibbs free energy (kJ/mol)
ΔH = change in enthalpy for the reaction (kJ/mol)
T = Temperature in Kelvins
ΔS = change in entropy for the reaction (kJ/mol K)

If ΔG = negative, then the reaction will occur spontaneously. If ΔG is a positive number, then the reaction will not be spontaneous.

A reaction at 298 K has a change in enthalpy of -80.7 kJ/mole and a change in entropy of -0.0963 kJ/mol K. Find the change in Gibbs free energy. Is the reaction spontaneous?

Solution
In this reaction, ΔH = -80.7 kJ/mole. Since ΔH is negative, energy is being released and the reaction will tend to be spontaneous. But, ΔS = -0.0963 kJ/mol K. A negative change in entropy means that the products are less random and more orderly, reducing the likelihood of spontaneity.

Substituting the values into the Gibbs free energy formula, we get

$\Delta G = \Delta H - T\Delta S$
$\Delta G = -80.7 - (298)(-0.0963)$
$\Delta G = -80.7 + 28.6974$
$\Delta G = -52.0$ kJ/mole.

Since ΔG is negative, the reaction will occur spontaneously.

Another way to calculate ΔG is to use a thermodynamic properties chart like the one below.

Thermodynamic Properties (at 25°C and 100.000 kPa)

ΔH_f° (kJ/mol) ΔG_f° (kJ/mol) S° (J/mol · K)
(concentration of aqueous solutions is 1*M*)

Substance	ΔH_f°	ΔG_f°	S°	Substance	ΔH_f°	ΔG_f°	S°
Ag(cr)	0	0	42.55	H_3PO_3(aq)	−964.4	—	—
$AgCl$(cr)	−127.068	−109.789	96.2	H_3PO_4(aq)	−1279.0	−1119.1	110.50
$AgCN$(cr)	146.0	156.9	107.19	H_2S(g)	−20.63	−33.56	205.79
Al(cr)	0	0	28.33	H_2SO_3(aq)	−608.81	−537.81	232.2
Al_2O_3(cr)	−1675.7	−1582.3	50.92	H_2SO_4(aq)	−909.27	−744.53	20.1
$BaCl_2$(aq)	−871.95	−823.21	122.6	$HgCl_2$(cr)	−224.3	−178.6	—
$BaSO_4$(cr)	−1473.2	−1362.2	132.2	Hg_2Cl_2(cr)	−265.22	−210.745	192.5
Be(cr)	0	0	9.50	Hg_2SO_4(cr)	−743.12	−625.815	200.66
BeO(cr)	−609.6	−580.3	—	I_2(cr)	0	0	116.135
Bi(cr)	0	0	56.74	K(cr)	0	0	64.18
$BiCl_3$(cr)	−379.1	−315.0	177.0	KBr(cr)	−393.798	−380.66	95.90
Bi_2S_3(cr)	−143.1	−140.6	200.4	$KMnO_4$(cr)	−837.2	−737.6	171.71
Br_2(l)	0	0	152.231	KOH(cr)	−424.764	—	—
CH_4(g)	−74.81	−50.72	186.264	$LiBr$(cr)	−351.213	—	—
C_2H_2(g)	+226.73	+209.20	200.94	$LiOH$(cr)	−484.93	−438.95	42.80
C_2H_4(g)	+52.26	+68.15	219.56	Mn(cr)	0	0	32.01
C_2H_6(g)	−84.68	−32.82	229.60	$MnCl_2$(aq)	−555.05	−490.8	38.9
CO(g)	−110.525	−137.168	197.674	$Mn(NO_3)_2$(aq)	−635.5	−450.9	218
CO_2(g)	−393.509	−394.359	213.74	MnO_2(cr)	−520.03	−465.14	53.05
CS_2(l)	+89.70	+65.27	151.34	MnS(cr)	−214.2	—	—
Ca(cr)	0	0	41.42	N_2(g)	0	0	191.61
$Ca(OH)_2$(cr)	−986.09	−898.49	—	NH_3(g)	−46.11	−16.45	192.45
Cl_2(g)	0	0	223.066	NH_4Br(cr)	−270.83	−175.2	113
Co_3O_4(cr)	−891	−774	—	NO(g)	+90.25	86.55	210.761
CoO(cr)	−237.94	−214.20	52.97	NO_2(g)	+33.18	+51.31	240.06
Cr_2O_3(cr)	−1139.7	−1058.1	81.2	N_2O(g)	+82.05	+104.20	219.85
$CsCl$(cr)	−443.04	−414.53	101.17	Na(cr)	0	0	51.21
Cs_2SO_4(cr)	−1443.02	−1323.58	211.92	$NaBr$(cr)	−361.062	—	—
CuI(cr)	−67.8	−69.5	96.7	$NaCl$(cr)	−411.153	−384.138	72.13
CuS(cr)	−53.1	−53.6	66.5	$NaNO_3$(aq)	−447.48	—	—
Cu_2S(cr)	−79.5	−86.2	120.9	$NaOH$(cr)	−425.609	—	—
$CuSO_4$(cr)	−771.36	−661.8	109	Na_2S(aq)	−447.3	—	—
F_2(g)	0	0	202.78	Na_2SO_4(cr)	−1387.08	−1270.16	149.58
$FeCl_3$(cr)	−399.49	—	—	O_2(g)	0	0	205.138
FeO(cr)	−272.0	—	—	P_4O_6(cr)	−1640.1	—	—
Fe_2O_3(cr)	−824.2	−742.2	87.40	P_4O_{10}(cr)	−2984.0	−2697.7	228.86
Fe_3O_4(cr)	−1118.4	−1015.4	146.4	$PbBr_2$(cr)	−278.7	−261.92	161.5
H(g)	+217.965	—	114.713	$PbCl_2$(cr)	−359.41	−314.10	136.0
H_2(g)	0	0	130.684	S(cr)	0	0	31.80
HBr(g)	−36.40	−53.45	198.695	SO_2(g)	−296.830	−300.194	248.22
HCl(g)	−92.307	−95.299	186.908	SO_3(g)	−454.51	−374.21	70.7
HCl(aq)	−167.159	−131.228	56.5	SrO(cr)	−592.0	−561.9	54.4
HCN(aq)	+150.6	+172.4	94.1	Ti(cr)	0	0	30.63
$HCHO$(g)	−108.57	−102.53	218.77	TiO_2(cr)	−939.7	−884.5	49.92
$HCOOH$(l)	−424.72	−361.35	128.95	TlI(cr)	−123.8	−125.39	127.6
HF(g)	−271.1	−273.2	173.779	UCl_4(cr)	−1019.2	−930.0	197.1
HI(g)	+26.48	+1.70	206.594	UCl_5(cr)	−1059	−950	242.7
H_2O(l)	−285.830	−237.129	69.91	Zn(cr)	0	0	41.63
H_2O(g)	−241.818	−228.572	188.825	$ZnCl_2$(aq)	−488.19	−409.50	0.8
H_2O_2(l)	—	−120.35	109.6	ZnO(cr)	−348.28	−318.30	43.64
H_3PO_2(l)	−595.4	—	—	$ZnSO_4$(aq)	−1063.15	−891.59	−92.0

We can use the chart to find ΔG for a reaction by putting ΔG_f values into the equation

$\Delta G = \sum \Delta G_f(\text{products}) - \sum \Delta G_f(\text{reactants})$

ΔG = change in Gibbs free energy for the reaction
$\sum \Delta G_f(\text{products})$ = sum of the change in Gibbs free energies of the products
$\sum \Delta G_f(\text{reactants})$ = sum of the change in Gibbs free energies of the reactants.

Using the thermodynamic properties chart, find ΔG for the reaction

$2BiCl_{3(cr)} + 3H_2S_{(g)} \rightarrow Bi_2S_{3(cr)} + 6HCl_{(g)}$

Solution

ΔG_f(products) (kJ/mole)	
$Bi_2S_{3(cr)}$	= -141
$HCl_{(g)}$ = -95.3 x 6	=-571
$\sum \Delta G_f$(products)	= -712.8

ΔG_f(reactants) (kJ/mole)	
$BiCl_{3(cr)}$ =-315 x 2	= -630
$H_2S_{(g)}$ = -33.6 x 3	= -100.8
$\sum \Delta G_f$(reactants)	= -730.8

Notice that we multiply the ΔG_f of each substance by the coefficient in front of it in the balanced equation. For example, the ΔG_f of HCl is multiplied by 6 since the balanced equation has 6HCl.

$\Delta G = \sum \Delta G_f(\text{products}) - \sum \Delta G_f(\text{reactants})$
$\Delta G = -712.8 - (-730.8)$
ΔG = 18 kJ/mole.
Since ΔG is positive, the reaction will not occur spontaneously.