

CH301 Worksheet 11 Answer Key: Thermodynamic Calculations for Chemical Reactions and Phase Changes

Check for explanation of solution key at bottom of page—Assume $T = 298\text{K}$. First describe the reaction below where it is written, then predict the sign for each answer and only then, do the calculation. The BE values are at the bottom of the worksheet. The formation constants are found in the textbook appendix and also as Worksheet 11a at <http://courses.cm.utexas.edu/dlaude/ch301/worksheetsf08.html>

This worksheet is painful at first, but once you get it you are a profoundly better chemist (and exam 3 test taker.)

Chemical Reaction	ΔH (kJ)	BE (kJ)	Δn_{gas}	w (kJ)= $-\Delta nRT$	Δn_{system}	$T\Delta S$ (kJ)	ΔG (kJ)
$\text{CH}_4\text{g} + 2\text{O}_2\text{g} \rightarrow \text{CO}_2\text{g} + 2\text{H}_2\text{Og}$ Combustion reaction, would predict large heat and spontaneous reaction. $\Delta n = 0$ means no work, small entropy change.	-802	-802	0	0	0	-1	-801
$2\text{H}_2\text{g} + \text{O}_2\text{g} \rightarrow 2\text{H}_2\text{Og}$ Spontaneous combustion reaction, would predict large heat. $\Delta n =$ negative which means entropy decreases	-484	-482	-1	+2.5	-1	-27	-458
$\text{C}_2\text{H}_5\text{OHl} + 3\text{O}_2\text{g} \rightarrow 2\text{CO}_2\text{g} + 3\text{H}_2\text{Og}$ Spontaneous combustion reaction, would predict large heat. $\Delta n =$ is positive so work on surroundings and positive entropy.	-1234	-1248	2	-5	1	66	-1300
$\text{C}_2\text{H}_5\text{OHl} + 3\text{O}_2\text{g} \rightarrow 2\text{CO}_2\text{g} + 3\text{H}_2\text{Ol}$ Combustion reaction, would predict large heat and spontaneous reaction. But a liquid is formed, so negative entropy change	-1366	-1248	-1	2.5	1	-41	-1325
$\text{C}_3\text{H}_8\text{g} + 5\text{O}_2\text{g} \rightarrow 3\text{CO}_2\text{g} + 4\text{H}_2\text{Og}$ Spontaneous combustion reaction, would predict large heat. $\Delta n =$ is positive so work on surroundings and positive entropy..	-2043	-2012	+1	2.5	1	31	-2074
$4\text{H}_2\text{Og} + 3\text{CO}_2\text{g} \rightarrow \text{C}_3\text{H}_8\text{g} + 5\text{O}_2\text{g}$ This is the reverse of a combustion reaction. So we know that it has the opposite signs from the example above and is consequently endothermic and unfavorable entropy	2043	+2012	-1	2.5	-1	-31	+2074
$\text{CCl}_4\text{l} \rightarrow \text{Cs} + 2\text{Cl}_2\text{g}$ This is a non-spontaneous process in which dry cleaning fluid would be expected to decompose into carbon and release chlorine gas. Not a likely event. The reaction has a highly favorable entropy so it must be endothermic.	135	860	2	-5	2	70	65
$\text{Ba}(\text{OH})_2(\text{H}_2\text{O})_8\text{s} + 2\text{NH}_4\text{NO}_3 \rightarrow \text{Ba}(\text{NO}_3)_2\text{s} + 2\text{NH}_3\text{g} + 10\text{H}_2\text{Ol}$ This is the reaction involving two white solids I do all the time. The process is spontaneous from experience. It is a highly endothermic process as we can tell from the cold temperature generated. The fact that ammonia is released as a gas indicates that the reaction spontaneity is driven by the large positive entropy.	NA	NA	2	-5	10	NA	NA
$2\text{O}_3\text{g} \rightarrow 3\text{O}_2\text{g}$ This reaction is spontaneous. It should have a small exothermic value and a favorable entropy change.	-286	Resonance, no BE	1	-2.5	1	41	-327

$\text{H}_2\text{O}_s \rightarrow \text{H}_2\text{O}_g$ Phase change from solid to gas. Expect temp. dependent spontaneity. From experience, spontaneous at room temperature. Reaction is endothermic, so the reaction spontaneity depends on positive entropy.	NA	NA	0	0	0	NA	NA
$\text{CO}_2g \rightarrow \text{CO}_2s$ This is a deposition reaction as a gas becomes a solid. At room temperature we know this is not spontaneous. Since the reaction must be exothermic (heat leaves the system as the dry ice is formed, the entropy must be sufficiently negative at room temperature to keep the reaction from occurring.	NA	NA	-1	2.5	0	NA	NA
$\text{NH}_3g + \text{HClg} \rightarrow \text{NH}_4\text{Cls}$ We have seen that this is a spontaneous reaction that generates a white solid from the reaction of the gas vapors. Since the entropy change is clearly negative, a large ΔH must contribute to spontaneity.	-176	NA	-2	5	-1	-85	-91
$2\text{H}_2\text{O}_{2l} \rightarrow 2\text{H}_2\text{O}_l + \text{O}_2g$ From experience, this reaction is spontaneous. Reaction heat is not large but positive entropy contributes to spontaneity.	-196	-352	1	-2.5	1	38	-234

Explanation of my solution key:

Here is the answer key for the thermodynamic worksheet--note that for the tables we used sometimes there was no data available so no calculation was done. First note descriptions of the reactions and the qualitative explanations in which the sign of the thermodynamic process is predicted. This is then supported by performing the calculation. I was right every time!! Also note that when all species are in the gas phase, the BE calculation is pretty close. But when other phases are involved, the energy change for the phase transition is not considered and the BE calculation is poor. In cases where an ionic bond was involved, no BE calculation was done. Also note that I didn't simply calculate ΔS but also multiplied it by 300 to get $T\Delta S$ with units of kJ. One more thing, I use as few digits as possible to make the calculation simpler. So I use 300K, not 298K, and I also rounded off the table data on occasion. Amazingly (not), I still am within a kJ on everything. Finally, one great way to find out if you have done these calculations correctly is to compare the ΔG_f calculation with the $\Delta H_f - T\Delta S_f$ calculation of ΔG_f . If they are the same it means that is internal consistency in the calculation—makes you feel warm all over.

Bond Energy Table (in addition, assume C=O is 799 kJ/mol for carbon dioxide)

TABLE 6.8 Mean Bond Enthalpies (kJ·mol⁻¹)

Bond	Mean bond enthalpy	Bond	Mean bond enthalpy
C—H	412	C—I	238
C—C	348	N—H	388
C=C	612	N—N	163
C \equiv C*	518	N=N	409
C=O	837	N—O	210
C—O	360	N=O	630
C=O	743	N—F	195
C—N	305	N—Cl	381
C—F	484	O—H	463
C—Cl	338	O—O	157
C—Br	276		

*In benzene.

Thermodynamic Data for Chemical Compounds Including Formation Data is found at

<http://courses.cm.utexas.edu/dlaude/ch301/worksheetsf08.html>

