

### Thermodynamic Reaction Solution Key

Check for explanation of solution key at bottom of page—assume room temperature for TDS calculation.

Chemical Reaction	$\Delta H$ (kJ)	BE (kJ)	$\Delta n_{\text{gas}}$	w (kJ)= $-\Delta nRT$	$\Delta n_{\text{system}}$	$\Delta S$ (kJ)	$\Delta G$ (kJ)
$\text{CH}_{4\text{g}} + 2\text{O}_{2\text{g}} \rightarrow \text{CO}_{2\text{g}} + 2\text{H}_2\text{O}_{\text{g}}$ 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
$2\text{H}_{2\text{g}} + \text{O}_{2\text{g}} \rightarrow 2\text{H}_2\text{O}_{\text{g}}$ Spontaneous combustion reaction, would predict large heat. $\Delta n =$ negative which means entropy decreases and work on system	-484	-482	-1	+2.5	-1	-27	-458
$2\text{H}_2\text{O}_{\text{g}} \rightarrow 2\text{H}_{2\text{g}} + \text{O}_{2\text{g}}$ This is the non-spontaneous reaction that only occurs when I throw a battery into water to produce $\text{H}_2$ gas. Values are opposite same magnitude but opposite signs of combustion reaction above.	484	482	1	-2.5	1	27	458
$\text{C}_2\text{H}_5\text{OH}_{\text{l}} + 3\text{O}_{2\text{g}} \rightarrow 2\text{CO}_{2\text{g}} + 3\text{H}_2\text{O}_{\text{g}}$ 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
$\text{C}_2\text{H}_5\text{OH}_{\text{l}} + 3\text{O}_{2\text{g}} \rightarrow 2\text{CO}_{2\text{g}} + 3\text{H}_2\text{O}_{\text{l}}$ Combustion reaction, would predict large heat and spontaneous reaction. But a liquid is formed, so there is a negative entropy change.	-1366	-1248	-1	2.5	1	-41	-1325
$\text{C}_3\text{H}_{8\text{g}} + 5\text{O}_{2\text{g}} \rightarrow 3\text{CO}_{2\text{g}} + 4\text{H}_2\text{O}_{\text{g}}$ Spontaneous combustion reaction, would predict large heat. $\Delta n =$ is positive so there is work on surroundings and positive entropy change.	-2043	-2012	1	-2.5	1	31	-2074
$4\text{H}_2\text{O}_{\text{g}} + 3\text{CO}_{2\text{g}} \rightarrow \text{C}_3\text{H}_{8\text{g}} + 5\text{O}_{2\text{g}}$ This is the reverse of the combustion reaction. So we know that it has the opposite signs from the example above and is consequently endothermic and unfavorable entropy change.	2043	+2012	-1	2.5	-1	-31	+2074
$\text{CCl}_{4\text{l}} \rightarrow \text{C}_{\text{s}} + 2\text{Cl}_{2\text{g}}$ This is a non-spontaneous process in which dry cleaning fluid would be expected to decompose at room temperature 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
$\text{Ba}(\text{OH})_2(\text{H}_2\text{O})_{8\text{s}} + 2\text{NH}_4\text{NO}_3 \rightarrow \text{Ba}(\text{NO}_3)_2\text{s} + 2\text{NH}_{3\text{g}} + 10\text{H}_2\text{O}_{\text{l}}$ 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 But positive	NA But positive	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	NA	1	-2.5	1	41	-327

$\text{H}_2\text{O}_s \rightarrow \text{H}_2\text{O}_l$ 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	negative at room temp
$\text{CO}_{2g} \rightarrow \text{CO}_{2s}$ 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 change must be sufficiently negative at room temperature to keep the reaction from occurring.	NA	NA	-1	2.5	0	NA	positive at room temp
$\text{NH}_3g + \text{HCl}g \rightarrow \text{NH}_4\text{Cl}s$ 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 negative $\Delta H$ 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. Most of the calculations were done in a dark parking lot using the dome light of a 5 year old Saturn, so take the answers with a grain of salt, and e-mail me if you find a problem. In the first column I have given qualitative explanations in which the sign of the thermodynamic process is predicted. As you can tell from the calculations, I was right every time!! In some cases the lack of Appendix K data kept me from performing a calculation. 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 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  $\Delta S$  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 never looked at the Appendix K data after the decimal. 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  $\Delta G_f$  calculation with a separate  $\Delta H - T\Delta S$  calculation of  $\Delta G$ . If they are the same it means that even though you may have done the work in a darkened parking lot, there is internal integrity in the calculation—makes you feel warm all over.