Journal of Physics Special Topics

P5_11 Water into Wine

Benedict Irwin, Peter Hicks, Hannah Lerman

Department of Physics and Astronomy, University of Leicester, Leicester, LE1 7RH.

November 13, 2013

Abstract

In the Gospel of John, Jesus turns a substantial quantity of water into wine. We investigate the change in enthalpy across a candidate reaction and determine it to be 1255kJmol^{-1} indicating an endothermic reaction. We then find the change in entropy to be 4.21kJmol^{-1}K^{-1} and calculate the energy required for the whole reaction to be 0.25-0.37GJ.

Introduction

In the Gospel of John (2 : 1-11) Jesus turns a substantial quantity of water into wine from two large stone vats [1]. We set out to calculate whether such a conversion is both chemically and physically possible, and the energy required to perform such a miraculous feat.

Water into Wine

We assume pure water is turned into a basic form of wine; water mixed with ethanol. We also assume the strength of this wine is 12% ABV. John 2:6 states that the quantity of water converted was '$20-30$ gallons' [1], assuming these are imperial gallons this equates to approximately $90-135$ litres of water. We assume the water is pure H_2O.

The conversion from water which contains only hydrogen and oxygen to ethanol which contains hydrogen, oxygen and carbon will clearly require a source of carbon. We assume the most likely source would be ambient carbon dioxide in the air. It is then possible to set up the reaction

$$3H_2O_{(l)} + 2CO_{2(g)} \rightarrow C_2H_6O_{(l)} + 3O_{2(g)}, \qquad (1)$$

which conserves the number of each type of atom. This reaction is occurring under standard pressure and temperature, $1atm$ and $298K$. To check whether this reaction would spontaneously occur we evaluate the overall change in bond enthalpy H [2],

$$\Delta H_{tot} = 3\Delta H_{H_2O} + 2\Delta H_{CO_2} - \Delta H_{C_2H_6O} - 3\Delta H_{O_2}, \qquad (2)$$

where the positive terms are the change in enthalpy required to break bonds (from the reactants) and negative terms are the enthalpy liberated due to bonds formed (in the products). If ΔH_{tot} is negative, more energy is liberated from forming the new bonds than is required to initially break the original bonds. In this case a chain reaction will occur spontaneously; an exothermic reaction. However, if ΔH is positive the reaction will be endothermic and will require a heat input from the surroundings. Normally, equation 2 would also require a small to moderate activation energy as not every pair of molecules that collide react. However, if one adds a catalyst to the system this activation energy is reduced. For simplicity we assume that Jesus is able to provide the 'perfect catalyst' to the reaction to make the additional activation energy negligible.

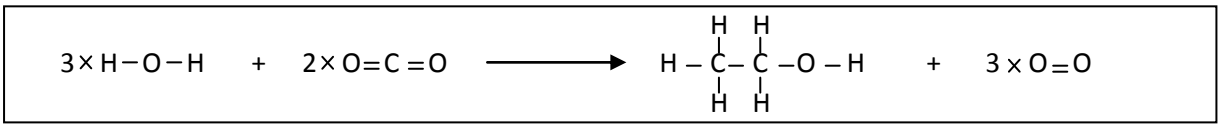

Figure 1: Bond displayed version of equation 1 showing single (-) and double bonds (=) between atoms.

Displaying equation 1 with all bonds shown gives figure 1. Using figure 1 and the values shown in table 1 we calculate ΔH to be $1255kJ/mol$, hence the reaction is endothermic and would not occur spontaneously. This is logical as the reverse of equation 1 is the burning of pure ethanol, an exothermic reaction.

Bond Type	Bond Enthalpy (kJ/mol)		Species	ΔH (kJ/mol)
$O-H$	463		H_2O	926
$C-H$	413		CO_2	1598
$C-O$	358		C_2H_6O	3234
$C=O$	799		O_2	495
$C-C$	348		-	-

Table 1: Tabulated values of individual bond enthalpies and those calculated for the reactants and products of Equation 1. [2]

Calculating the Entropy

We can now calculate the change in entropy caused by the reaction. In thermodynamics enthalpy is defined as [3]

$$H(S,p) = U + pV, \qquad (3)$$

with S the entropy, p the pressure per mol, U the internal energy and V the volume of the system. A change in Enthalpy is therefore

$$\Delta H = \Delta U + \Delta pV + p\Delta V, \qquad (4)$$

The combined law of thermodynamics is [3]

$$\Delta U = T\Delta S - p\Delta V, \qquad (5)$$

where T is the temperature of the system. Substituting Equation 5 into Equation 4 yields

$$\Delta H = T\Delta S + \Delta pV, \qquad (6)$$

During the reaction the vats of water are open to the air. The change in pressure of the atmosphere due to the reaction would be negligible, therefore we use the isobaric approximation $\Delta p = 0$. Equation 6 then leaves the relation,

$$\Delta H = T\Delta S. \ (7)$$

At a temperature of $298K$ equation 7 gives a change in entropy of $\Delta S = 4.21kJmol^{-1}K^{-1}$. A fundamental theorem of thermodynamics is that the entropy of a closed system never decreases, however as the entropy does increase with the reaction it is physically allowed in a closed or open system [3].

To calculate the total energy required to convert the reagents into their products we find the number of moles of water that require conversion. Using

$$n = \frac{m_g}{M}, \qquad (8)$$

where m_g is the mass of substance in grams, n is the number of moles and M is the molar mass of the substance, we find that 12% of the original $90-135$ litres of water (the volume that will go to make alcohol), at a molar mass of $18gmol^{-1}$ and mass of $1kgL^{-1}$ gives $600-900mol$ of water. Due to equation 1, $2mol$ of CO_2 is required for every $3mol$ of H_2O. Therefore $400-600mol$ of CO_2 are required for the reaction.

From the values in Table 1 the sum of the energies to break up these quantities of chemicals into their atomic constituents will be, $1.19GJ\ to\ 1.79GJ$. Liberating the bond energy for $600-900mol$ of diatomic oxygen and $200-300mol$ of ethanol; $0.94GJ\ to\ 1.42GJ$. This means Jesus would have to supply $0.25GJ-0.37GJ$ of energy to the reaction to keep it sustained.

Conclusion

The reaction outlined is endothermic and will not chemically proceed spontaneously. However, such a reaction leads to an increase in entropy of the system and is physically allowed. The input of $0.25GJ-0.37GJ$ of energy is a significant task and this is still under the assumption of a perfect catalyst, thus without additional equipment the extract from John does remain a miracle.

References

[1] - John 2:1-11 – The Bible, New International Version (NIV)
[2] - http://www.kentchemistry.com/links/Kinetics/BondEnergy.htm, Last accessed 12/11/2013
[3] - Thermodynamics, Kinetic Theory and Statistics. F. Sears, G. Salinger, 3rd Edition.