**Elimination Kinetics: Measuring the Rate and Yield of E2 Eliminations**

**Discussion and Results**

In conclusion, this particular lab experiment’s main purpose was to perform E2 and/or SN2 on a variety of alkyl halides.

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| Substrate | Trial | Theoretical yield (mol) | Theoretical Yield (mL) | Actual Yield (mL) | %  Yield | Ratio SN2:E2 | K1 (1/s) | K2 (1/Mols) |
| Bromoethane | 1 | 0.00207 | 60.8 | 5.7 | 9.4 | 9.67 | 0.00862 | 0.00165 |
| 2 | 0.00178 | 52.1 | 7.0 | 13.4 | 6.44 | 0.00777 | 0.00149 |
| 1-bromobutane | 1 | 0.00103 | 30.2 | 5.0 | 16.5 | 5.05 | 0.00883 | 0.00176 |

*Bromoethane*

Trial 1 and 2, both indicate that the SN2 reaction is more favorable than an E2 reaction, evidence from the ratios= 9.67:1 (T1) and 6.44:1 (T2). The only way that an E2 reaction would be favored, is if it could create a branched alkene (A branched alkene is stabilizes the reaction at its transition state, an a more stable transition state indicates a more favorable E2 reaction to occur than SN2. Although, since no branched alkene could be formed for the reaction between bromoethane and potassium hydroxide (only having 2 carbons), then the most favorable one would be an SN2 reaction. In addition, since the alkane is a very strong base @ pka = 50 and the hydroxide @ pka=15, thus requiring a huge amount of energy resulting in the low percent yields of the two trials: 9.4% (T1) and 13.4%(T2). An SN2 is favored because the Bromine and the hydroxide (from the KOH) undergo a single step, in which bromine is being replaced by the hydroxide leading to a more stable transition state (with less energy required). In a general sense, most primary alkyl halides undergo an SN2 reaction mechanism. Furthermore, Bromine is an excellent leaving group considering that it is from 4th period with a large atomic radius. Hence, bromine being a primary alkyl halide, a good leaving group and nucleophile, leads to a more favorable SN2 reaction than an E2.

*1-Bromobutane*

Due to lack of time, only one trial was conducted with this substrate. Thus, Trial 1 indicate that an SN2 mechanism was also more favorable than E2 mechanism, with the evidence regarding rations= 5.05:1 (T1). The explanation for this reaction is similar to the one of Bromoethane as both are un-branched alkanes. Although Bromobutane can form a branched alkene but that would be a very unstable reaction in the transition state. Thus, Bromine being an excellent leaving group with a large atomic radius, a primary alkyl halide, and a good nucleophile, leads to a more favorable SN@ reaction than E2. However, the reason why the ratio is lower than that of bromoethane is because there is a larger possibility of creating a branched alkene through a E2 reaction due to the

*Reaction Rates*

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| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Substrate | Trial | Mass of KOH  (g) | [KOH]  (M) | Theoretical yield (mol) | %  Yield | Ratio SN2:E2 | K1 (1/s) | K2 (1/Mols) |
| Bromoethane | 1 | 0.7351 | 5.24 | 0.00207 | 9.4 | 9.67 | 0.00862 | 0.00165 |
| 2 | 0.7334 | 5.23 | 0.00178 | 13.4 | 6.44 | 0.00777 | 0.00149 |
| 1-bromobutane | 1 | 0.7044 | 5.02 | 0.00103 | 16.5 | 5.05 | 0.00883 | 0.00176 |

Both trials for bromoethane consist of 5.24M and 5.23M of KOH with 9.4% and 13.4% yield; these values have a very tiny difference, which could be a result of procedural error. Since they both were an SN2 reaction, it is a second order reaction. Thus, having the concentrations of both KOH affecting the rate of reaction. Hence, even though they have different percent yields, the K2 are quiet similar with 0.00165/Mols and 0.00149/Mols. Similar theory can be applied for the substrate 1-bromobutane.

*Some limitations for this lab experiment could be that between 0-30s it’s very tough to get both of the burets leveled as the gas increased and decreases the volume very fast. Thus, there could be enormous amount of uncertainty with the values at the very beginning. Also, while leveling both of the burets, it was done by the human eye, which carries its own uncertainty. If this lab was to be done accurately, a machine should’ve done it.*