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# Soft drinks catalyzed hydrolysis and alcoholysis of epoxides

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## ABSTRACT

Commonly consumed soft drinks have been utilized for the first time for the efficient hydrolysis and alcoholysis of epoxides furnishing the corresponding 1,2-diols and $\alpha$-alkoxyalcohols respectively.

KEYWORDS

Soft drinks;
Hydrolysis;
Alcoholysis;
Epoxides.

## INTRODUCTION

Epoxides are versatile synthetic intermediates for organic synthesis and they undergo wide variety of nucleophilic ring opening reactions. There have been several studies reported on the epoxide ring opening with wide variety of nucleophiles under a plethora of conditions[1] such as protic/Lewis acids, homo- and heterogeneous metal catalysis, ionic liquids, solid and aqueous phase reactions, etc. While each method has its own merits and limitations, there is still a need for the development of highly simplified and environmentally benign procedures without the use of any toxic/expensive catalysts or harsh reaction conditions.

Organic solvents are used extensively in the industry as well as in the academic labs, and their release into the environment is a matter of immense health and safety concern. Due to the wide range of hazards that are associated with these volatile organic compounds, there have been tremendous efforts towards finding clean alternative sources. Beverages such as Coca-Cola®[2], Pepsi®[3], etc. are highly inexpensive and extensively consumed all over the world. These type of soft drinks are mildly acidic[4], however they have never been used for any type of reactions for organic synthesis. Accordingly, we envisioned the use of these drinks for acid mediated synthetic organic transformations.

## EXPERIMENTAL

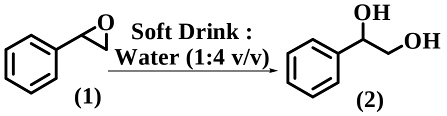
### Hydrolysis of epoxide with coke

To a solution of 5mL Coke (or a 20% v/v solution of Coke in water) was added 240 mg (2mmol) of styrene oxide, and stirred for two hours at room temperature. Upon completion (TLC), the reaction mixture was diluted with saturated brine (5mL) and worked up ethyl acetate (3×20 mL), dried ($MgSO_4$), and concentrated in vacuo to obtain spectroscopically pure diol (257mg, 93% yield).

### Alcoholysis of epoxide with coke

To a solution of the methanol (4.5 mL) and styrene oxide (240 mg, 2mmol) was added 10% v/v (0.5 mL) of Coca-Cola, and stirred at 50°C overnight. Upon complete consumption of the epoxide (TLC), the reaction mixture was concentrated in vacuo, diluted with

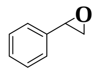
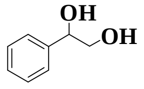
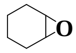
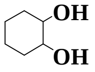
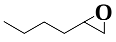
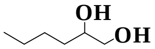
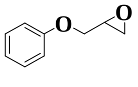
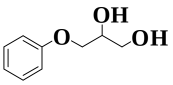
**TABLE 1: Hydrolysis of styrene oxide in various soft-drinks**



| | Soft Drink | Amount (v/v) | Time (h) | Diol yield (%) |
|---|---|---|---|---|
| 1 | Coca cola®[2] | 100 | 2 | 95 |
| 2 | Coca cola® [2] | 20 | 2 | 93 |
| 3 | Diet coke® [2] | 20 | 2 | 88 |
| 4 | Pepsi® [3] | 20 | 2 | 92 |
| 5 | Sprite® [3] | 20 | 2 | 93 |
| 6 | Mountain dew® [3] | 20 | 2 | 89 |
| 7 | Fanta® [2] orange | 20 | 2 | 87 |
| 8 | Barq's® [2] root beer | 100 | 24 | 91 |
| 9 | Barq's® [2] root beer | 20 | 24 | 90 |
| 10 | Canada dry® [5] club soda | 100 | 168 | 20$^a$ |

$^a$20% of the diol was obtained along with remaining starting material even after stirring for one week

**TABLE 2: Hydrolysis of epoxides with Coca Cola®**

| Sr. no. | Epoxide | Coca Cola (v/v) | Product | Temp (°C) | Time (h) | Yiel (%) |
|---|---|---|---|---|---|---|
| 1 |  | 100% |  | 25°C | 2 | 95 |
| 2 | - | 20% | - | 25°C | 2 | 93 |
| 3 |  | 100% |  | 25°C | 24 | 96 |
| 4 | - | 20% | - | 25°C | 24 | 93 |
| 5 |  | 100% |  | 25°C | 24 | 95 |
| 6 | - | 20% | - | 25°C | 24 | 41 |
| 7 | - | 20% | - | 50°C | 12 | 68 |
| 8 |  | 100% |  | 25°C | 48 | NR |
| 9 | - | 100% | - | 50°C | 12 | 98 |

saturated brine (5mL) and worked up with ethyl acetate (3×20 mL) and water. The combined organic layers were dried ($MgSO_4$), and concentrated to obtain 17:1 mixture of alcohol and diol in 95% combined yield, based on crude proton NMR analysis.

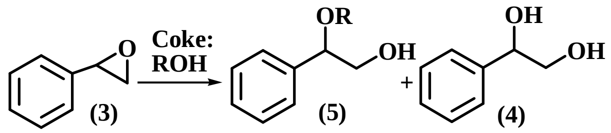
## RESULTS AND DISCUSSION

As a model study, we carried out the hydrolysis and alcoholysis of epoxides using soft drinks as catalysts. Initially, we attempted the reaction of styrene oxide **(1)** with Coca-Cola® Classic and gratifyingly, the hydrolysis took place smoothly at room temperature and the reaction was complete within 2h. A simple work up of the reaction furnished spectroscopically pure 1-phenyl-1,2-ethanediol **(2)** in 95% yield. Impressed by this result, we carried out the hydrolysis of **(1)** in 4:1 (v/v) solution of water and coke, and the hydrolysis was found to be equally facile and the product diol was obtained in 93% yield. The hydrolysis of **(1)** was then attempted in other commonly consumed soft drinks such as Pepsi®, Sprite®, Fanta® Orange, Mountain Dew®, Diet Coke®, and Barq's® Root Beer. The reaction was observed to be uniform in all the above cases and the diol was obtained in consistently high yields (entries 3-9, TABLE 1).

The comparatively less acidic soft drink Root Beer (pH~4.6) took longer time (24h) for completion of hydrolysis. The hydrolysis also took place in the presence of catalytic Root Beer in water as solvent (entry 9). Expectedly, the reaction of **(1)** with Club Soda (Canada Dry®, pH ~5.2) was sluggish and only ~20% hydrolysis took place even after stirring for one week (entry 10, TABLE 1).

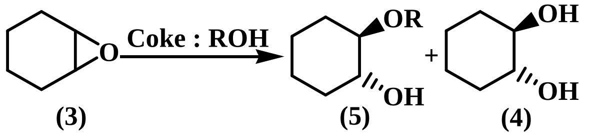
To further test the generality of this reaction, hydrolysis of several other representative epoxides such as cyclohexene oxide, 1,2-epoxyhexane and phenyl glycidyl ether was attempted using Coca Cola® Classic. In all these cases, the product diols were obtained in very high yields in stoichiometric Coke or in a solution of Coke in water (TABLE 2). Phenyl glycidyl ether was relatively sluggish to react at room temperature, and elevated temperature (50°C) was required to affect the hydrolysis (entries 8-9, TABLE 2).

We then studied the alcoholysis of epoxides using Coke as a catalyst in methanol, and ethanol. As a representative example, the reaction of styrene oxide was attempted with methanol in the presence of 20% v/v Coke to yield 2-methoxy-2-phenyl ethanol as a single regioisomer. However, hydrolysis was observed as a competitive side reaction from the water present in Coke and 3.3:1 ratio of alcohol to diol was obtained. To minimize the hydrolysis, the reaction was attempted with lower amount (10% v/v) of Coke, to affect the alcoholysis in 17:1 ratio. Lowering of the amount of Coke (5% v/v) led to slower rate of alcoholysis with no further improvement in chemoselectivity. Heating the reaction at 50°C in the presence of 5% v/v Coca-Cola



20% v/v Coke in MeOH, 25°C: 3.3 : 1
5% v/v Coke in MeOH, 25°C: 17 : 1
5% v/v Coke in MeOH, 50°C: 17 : 1
20% v/v Coke in EtOH, 25°C: 2.4 : 1
20% v/v Coke in EtOH, 50°C: 4.2 : 1

SCHEME 1: Alcoholysis of styrene oxide



20 % v/v Coke in MeOH, 50°C:1.5 : 1
20 % v/v Coke in EtOH, 50°C: 0.75 : 1

SCHEME 2: Alcoholysis of cyclohexene oxide

proved optimal for methanolysis, and the corresponding alcohol was obtained in 95% yield. The reaction of ethanol was observed to be slower than methanol and ~10% v/v Coke was required for complete consumption of epoxide at 50°C, and a 4.2:1 mixture of alcohol:diol was obtained in 94% yield (SCHEME 1).

Cyclohexene oxide proved even slower towards alcoholysis, and reaction of methanol and ethanol in the presence of 20% Coke provided a mixture of alcohol and diol in a ratio 1.5:1 and 0.75:1 respectively (SCHEME 2).

## CONCLUSIONS

In conclusion, we have developed an inexpensive and convenient procedure for the soft drinks catalyzed hydrolysis and alcoholysis of epoxides. We have demonstrated that a variety of epoxides undergo hydrolysis in nearly quantitative yields in the presence of various commonly consumed soft drinks. Similarly, we have also shown that alcohols undergo reaction with epoxides in the presence of catalytic amount of soft drinks. Owing to the inexpensive availability, general acceptance and environmental amicability of the soft drinks, the present methodology could open up a range of applications amongst the industry as well as in the academia.

## ACKNOWLEDGMENT

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[3] Pepsi®, and Mountain Dew® are registered trademarks of PepsiCo, Inc.

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[5] Canada Dry® is a registered trademark of Cadbury Beverages Inc.