KINETICS OF THE INVERSION REACTION OF SUGAR

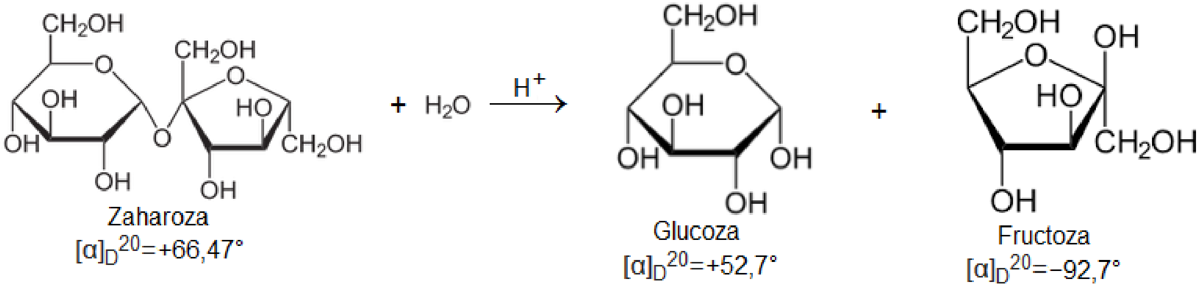
1. PURPOSE OF THE WORK

Determination of the rate constant and the reaction order for the inversion of sucrose in dilute aqueous solution in homogeneous acid catalysis.

2. THEORETICAL NOTIONS

The sucrose inversion reaction is, in fact, an acid-catalyzed hydrolysis in solution sufficiently diluted to satisfy the conditions of order degeneracy.

The chemical reaction is:



which, in dilute aqueous solution, follows a kinetic of order I described by the equation:

$$\ln \frac{C_Z^0}{C_Z} = kt$$

where the index Z refers to sucrose, the upper index 0 refers to the initial moment, and k represents the rate constant.

The above equation can also be reformulated in terms of other concentration-dependent linear quantities, such as the rotation angle of the plane of polarized light (the polarimetric angle) that depends on the concentration according to the *Lambert-Beer* law:

$$\alpha = [\alpha] \cdot l \cdot C$$

where α is the polarimetric angle, $[\alpha]$ is the specific polarimetric angle of the substance ("specific rotation"), l is the optical path length in cm (the length of the path traveled by the light beam through the solution), and C is the concentration of the solution.

In this case, however, the polarimetric method introduces an additional complication, because all the involved substances (except water) are optically active, so that the concentration cannot be replaced directly with the polarimetric angle. In order to obtain the correct relation, we will observe that the experimentally determined polarimetric angle is the sum of the rotation angles of the three optically active species and we will write successively:

$$\alpha = \alpha_Z + \alpha_G + \alpha_F =$$

$$= [\alpha]_Z l (C_Z^0 - x) + [\alpha]_F l x + [\alpha]_G l x =$$

$$= [\alpha]_Z l C_Z^0 - ([\alpha]_Z - [\alpha]_F - [\alpha]_G) l x$$

where x is the volumetric degree of advancement (specific advancement). The above equation is valid at any time from the reaction history, so also in the initial state (when the system contains only sucrose and water) and in the final state (when the system is a solution of fructose and glucose). Noting α_0 and with α_∞ to the polarimetric angles measured in these two states, we have:

$$\alpha_0 = [\alpha]_Z l C_Z^0, \qquad \alpha_\infty = ([\alpha]_F + [\alpha]_G) l C_Z^0$$

which leads to relation:

$$(\alpha_0 - \alpha) C_Z^0 = (\alpha_0 - \alpha_\infty) x$$

With these notations, the kinetic equation for first order reactions becomes successive:

$$kt = \ln \frac{C_Z^0}{C_Z^0 - x} = \ln \frac{1}{1 - \frac{x}{C_Z^0}} = \ln \frac{\alpha_0 - \alpha_\infty}{\alpha - \alpha_\infty}$$

or, more:

$$\ln(\alpha - \alpha_\infty) = kt + \ln(\alpha_0 - \alpha_\infty) \qquad (1)$$

which, in the coordinate system $(x, y) = (t, \ln(\alpha - \alpha_\infty))$, represents a linear model for the time dependence of the polarimetric angle. This model can be used to determine the apparent rate constant and to determine the reaction order for sucrose inversion.

3. EXPERIMENTAL PART

The principle of the method

A dilute acid solution of sucrose is analyzed polarimetrically, obtaining values of the polarimetric angle at various times in time, including the rotation angle corresponding to the final state, in which the sucrose is depleted. The data thus obtained are used to determine the quality of the correlation with the linear model above, thus determining the reaction order. The apparent rate constant results as a collateral product of the analysis.

We note that in this paper the diagnosis of regression is an essential stage, the quality of the correlation being an indicator of the order of reaction.

3.1. APPARATUS AND SUBSTANCES

- polarimeter, water bath, polarimetric tubes, three Erlenmayer glasses, 100 mL graduated cylinder, sugar, 1N HCl solution, 2N HCl solution, distilled water.

3.2. PROCEDURE

1. Prepare a solution of 20% (w / w) sucrose by dissolving 16 g of commercial sucrose (white crystallized sugar) in 64 mL of distilled water;
2. The obtained solution is divided into two parts of 35 mL, in two Erlenmeyer glasses;
3. Measure a volume of 35 mL of 1 M hydrochloric acid solution, pour over one of the sucrose solutions and shake, at which time the stopwatch for this solution is started.
4. Fill a polarimetric tube with the resulting solution and read the rotation angle, noting the time indicated by the stopwatch (**which should not be stoped**).
5. Repeat steps 3, 4 using a 2 M hydrochloric acid solution and the second sucrose solution.
6. The two Erlenmayer glasses with the solution residues are immersed in a thermostatic water bath at 85 ° C for about 10 minutes;
7. Read the polarimetric angle for each solution in 10 to 10 minutes compared to the first reading, for one hour;
8. The heated solutions in the water bath are brought to room temperature, then introduced into the two polarimetric tubes. Measure the two α_∞ corresponding values.

The polarimetric angle reading is done by rotating the drum under the polarimeter eyepiece until the field of view is completely black. At this point, the rotation angle can be read on the hinged disc as follows: the entire part is given by the division closest to the hinges grade 0, and the first decimal is given by the first division on the hinged one, which is in the extension of a division on the inner disk. Attention: angle fractions are expressed in tenths, not arc minutes.

4. EXPERIMENTAL DATA PROCESSING

4.1. Using the experimental data, fill in a table with the format below:

No.	t**, min**	α	$\alpha - \alpha_\infty$	$\ln(\alpha - \alpha_\infty)$
1				
…				

If the data are processed analytically, the parameters of the linear model (1) are determined for each series of measurements and the coefficient of determination is calculated. If this coefficient is greater than 0.95 it can be considered that the reaction follows a kinetic of order I whose apparent constant is given by the slope of the regression line.

If the data is graphically processed, the logarithm of the angle difference in the last column of the table is represented by time and the right regression is plotted. If the experimental points are linearly correlated (they are grouped around the regression line) then the apparent kinetics of the reaction is of the first order, and the velocity constant is given by the slope of the straight line.

Compare the slopes of the regression rights for the two sets of measurements and discuss the results.

5. QUESTIONS

5.1. What is the theoretical relationship between the slopes of the two regression lines assuming that the order is completely degenerate? Justify.

5.2. Calculate the molar ratio of sucrose: water and show that the water is excess enough to justify the order degeneracy hypothesis.

5.3. If the order had not been completely degenerate (the excess water would not have been sufficient), how would this have been reflected in the graph $\ln(\alpha - \alpha_{\infty}) = f(t)$? Justify.