# **Kinetics of the inversion of saccharose**



Der Reaktionsverlauf der Zucherinversion wird von einer Änderung des Drehwinkels für polarisiertes Licht begleitet. Während Glucose rechtsdrehend ist, dreht Invertzucker die Polarisationsebene linear polarisierten Lichts nach links. Die zeitliche Änderung des Drehwinkels von polarisiertem Licht wird mit Hilfe eines Halbschattenpolarimeters gemessen









# **General information**

### **Application**



Many biologically important substances are chiral. The different conformers can have very different functions in biological systems. Many cell receptors and enzymes are highly enantiomer-specific and are specialised in clockwise or counterclockwise connections. Almost all natural amino acids are therefore present in L-form, whereas the D-form predominates for sugars. A good example of stereoselectivity is the thalidomide scandal in the 1950s/60s. This sedative, which was popular at that time, was often used as a sedative for pregnant women. It was only after years of use that it was discovered that the Lform of the chiral molecule had a strong fruit-damaging effect, which led to numerous births of children with malformations. Only the R-form of thalidomide leads to Experimental setup the desired sedative effect.







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## **Theory (1/6)**

Optical activity is the ability of certain substances to rotate the plane of vibration of linearly polarised light. When linearly polarised light passes through such a substance, the radiation components are shifted in phase due to the interaction of substances which contain asymmetric carbon atoms. This phase shift is seen as a rotation of the plane of polarisation.

The specific rotation of optically active solutions is defined as that angle at which the plane of vibration of sodium-D-light ( $\lambda$  = 589.9 nm) is rotated when the thickness of the layer of the solution is 100 mm, 1 g of substance is dissolved in 1  $\text{cm}^3$ , and the measurement is undertaken at a temperature of 20 °C.

The angle of rotation  $\alpha$  is proportional to the concentration c of the dissolved substance.

The specific rotation [ $\alpha$ ]D can be so determined by testing solutions of known concentration:

$$
[\alpha]_{D}^{20} = \frac{\alpha}{c}
$$



PHY WE excellence in science **Theory (2/6)**



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If the temperature of measurement  $\vartheta$  deviates from 20 °C, the result can be converted to this temperature by using equation (2) for lactose and equation (3) for saccharose:

$$
[\alpha]_D^{20}\,=\,[\alpha]_D^{\vartheta}\,-\,0.072\cdot(20\degree{\rm C}\,-\,\vartheta)
$$

$$
[\alpha]^{20}_{D}\,=\,\frac{[\alpha]^{\vartheta}_{D}}{1\,-\,0.00037\,\left(\vartheta\,-\,20\degree \text{C}\right)}
$$

In an acidic environment, saccharose undergoes hydrolytic cleavage into glucose and fructose, in a process catalysed by oxonium ions.

## **Theory (3/5)**

Dextrorotatory saccharose is converted into dextrorotatory glucose and laevorotatory fructose.

 $\text{success} \quad + \quad \text{H}_2\text{O} \quad \rightarrow ^{[\text{H}_3\text{O}^+]} \quad \text{glucose} \quad + \quad \text{fructose}$  $[\alpha]_D^{20} = +66.5$ °  $[\alpha]^{20}_{\not\!\!D}=+52\degree\qquad [\alpha]^{20}_{\not\!\!D}=-92\degree$ invert sugar

Overall, this reaction corresponds to a pseudo-first order reaction, i.e. the reaction rate depends only on the saccharose concentration.

$$
-\frac{\mathrm{d}c}{\mathrm{d}t} = k \cdot c
$$

The rate of reaction is defined as the change in concentration  $dc$  per unit of time  $dt$ .



## **Theory (4/6)**

The reaction rate decreases with the concentration  $c$ . The proportionality factor of this relationship is the rate constant  $k$ , which is characteristic for a specific reaction. Integration of the last equation results in:

$$
\ln\frac{c_0}{c} \,=\, k\,\cdot\,(t\,-\,t_0)
$$

where  $c_0$  is the initial concentration at time  $t_0 = 0$  and  $c(t)$  is the concentration at time  $t$ .

A change of the concentration corresponds to a change of the angle of rotation.

$$
\ln\frac{c_0}{c} = \ln\frac{\alpha_0 - \alpha_\infty}{\alpha_t - \alpha_\infty}
$$

where  $\alpha_t$  is the angle of rotation at time  $t$ ,  $\alpha_0$  is the angle of rotation of pure saccharose solution and  $\alpha_\infty$  is the angle of rotation when hydrolysis has been completed.

### **Theory (5/6)**

Taking the last two equations into account, it follows that

$$
k = \frac{1}{t} \cdot \ln \frac{\alpha_0 - \alpha_\infty}{\alpha_t - \alpha_\infty}
$$

k can also be calculated from the slope  $\frac{1}{h}$  of the straight line resulting from k

$$
t\,=\,\frac{1}{k}\,\cdot\,\ln\frac{\alpha_0\,-\,\alpha_{\infty}}{\alpha_t\,\,\alpha_{\infty}}
$$

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### **Equipment**







# **Setup and procedure**







Put up a tripod stand (shown in the pictue) and put the waterbath next to it that the clamp (to fix the tube of the polarimeter) is positioned in the waterbath.

Take the waterbath and fill it with water until the heating system is complete covered with water.

Programme the waterbath temperature at 30°C



### **Setup (2/3)**

- $\circ$  Prepare the solutions required for the experiment as follows:
- **2 molar HCl solution**: Pour the contents of the ampoule (for 1 l of 1 M hydrochloric acid) into a 500 ml volumetric flask and fill up to the calibration mark with distilled water.
- **Saccharose solutions:** Weigh 12.000 g of saccharose into a 50 ml volumetric flask, dissolve it in distilled water, and fill up to the calibration mark with distilled water (c = 0.24 g/  $\rm cm^3$ ). Transfer the solution into a 100 ml beaker. Pipette 10 ml of the solution into a second glass beaker and add 10 ml of water (c/2). Prepare solutions of concentrations c/4 and c/8 by pipetting 10 ml each of the c/2 and c/4 solutions into two further glass beakers and adding 10 ml of water.
- **Lactose solutions:** Weigh 1.500 g of lactose into a 50 ml volumetric flask, dissolve it in distilled water, and fill up to the calibration mark with distilled water (c = 0.030 g/  $\rm cm^3$ ). Prepare solutions of concentrations c/2, c/4 and c/8 from this as for saccharose.



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### **Procedure (1/3)**



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### **Angle measurement First experiment part - Determination of**  $α_0$ .

To investigate the kinetics of saccharose inversion, warm the saccharose solution of concentration  $c =$ 0.24 g/cm $3$  and the 2 molar hydrochloric acid solution to 30 °C in the temperaturecontrolled bath.

Pipette 20 ml of the warm saccharose solution into a 100 ml beaker and add 20 ml of destillied water.

Fill the polarimeter cell bubble-free with the saccharose solution and hang it into the thermostatic bath.

Warm the polarimeter cell at least for 5 minutes.

Remove the cell from the bath, dry its exterior surface, and after exactly 5 minutes determine the angle of rotation  $\alpha_0$ .

### **Procedure (1/3)**



To investigate the kinetics of saccharose inversion, warm the saccharose solution of concentration c  $= 0.24$  g/cm<sup>3</sup> and the 2 molar hydrochloric acid solution to 30 °C in the temperaturecontrolled bath.

Pipette 10 ml of the warm saccharose solution into a 100 ml beaker and add 10 ml of hydrochloric acid.

Start the stopwatch.

Fill the polarimeter cell bubble-free with the acidified saccharose solution and hang it into the thermostatic bath.

In due good time remove the cell from the bath, dry its exterior surface, and after exactly 5 minutes determine the angle of rotation  $\alpha_t$ .



### **Procedure (3/3)**

### **Third experiment part - Determination of**  $( \alpha_{\infty} )$ .

Again temperature equilibrate the cell and take a value every 5 minutes, following the same procedure as in part one. Stop the measurement series after 50 minutes.

Parallel to this, mix 10 ml saccharose solution of concentration  $c = 0.24$  g/ $cm<sup>3</sup>$  and 10 ml of 2 molar hydrochloric acid solution in a 100 ml beaker and heat it to 70 °C on a magnetic heating stirrer, using a 600 ml beaker as water bath.

After 10 minutes, temperature equilibrate it in the thermostatic bath to 30 °C and then measure the angle of rotation ( $\alpha_{\infty}$ ).





# **Evaluation**



**Evaluation (1/5)**

**Determine the rate constant of the inversion of saccharose !**





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The figure shows the experimental values obtained for  $c_0 = 0.12 \frac{g}{cm^3}$  and 30 °C.

$$
t\,=\,\frac{1}{k}\,\cdot\,\ln\frac{\alpha_0\,-\,\alpha_{\infty}}{\alpha_t\,\,\alpha_{\infty}}
$$

They result in a rate constant of  $k ~=~ 2.5 \, \cdot \, 10^{-2} \, \mathrm{min}^{-1}$  .



### **Evaluation (3/5)**

### **Name all parameters that influence the optical rotation!**

The magnitude of the optial rotation is affected by...

### **Evaluation (4/5)**





### **Evaluation (5/5)**

### **Which processes do you know for the production of polarized light?**

