Measuring the Optical Rotation of Chiral Molecules

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L2 Lab Skills, PH228, Tuesday

This experiment measured the optical rotation of sucrose, glucose, and fructose solutions using a polarimetric setup at 520nm. Specific rotations were found to be $+89.7 \pm 1.0°$, $-122.8 \pm 1.4°$, and $+138.8 \pm 1.6°$, respectively. These values deviated substantially from literature values reported at the sodium D-line (589nm). Applying a dispersion correction via Drude's equation, the inferred D-line rotations were $+68.62 \pm 0.77°$ for sucrose and $+106.70 \pm 1.23°$ for glucose. The sucrose result matched literature within uncertainty, while glucose remained anomalously high, and no correction was possible for fructose due to missing parameters. This deviation is consistent with mutarotation in glucose, which may not have reached equilibrium before measurement.

I. Introduction

Optical rotation is a classical phenomenon with enduring practical applications. It is used in chemistry, biology, and industry to assess the concentration and purity of chiral substances, particularly sugars, amino acids, and pharmaceutical compounds. Polarimetry offers a non-destructive and precise method for measuring this, and remains in widespread use for routine quality control and analytical diagnostics.

Chiral molecules lack mirror symmetry and interact asymmetrically with circularly polarised light. When linearly polarised light enters such a medium, its left- and right-circularly polarised components experience different refractive indices. The resulting phase shift between these components leads to a net rotation of the polarisation plane, which can be measured as the light exits the medium.

The specific rotation $[\alpha]_\lambda^T$ at a given temperature T and wavelength λ is defined as:

$$[\alpha]_\lambda^T = \frac{\alpha}{l \times c} \qquad (1)$$

where α is the observed rotation angle, l is the path length in decimetres, and c is the concentration of the solution in grams per millilitre of solution [3].

A fundamental principle in optical rotation measurements is Malus' law, which describes the intensity of light passing through a polariser as a function of angle between the polarisation direction and the polariser's transmission axis θ.

$$I = I_0 \cos^2 \theta \qquad (2)$$

This relationship allows the rotation angle to be extracted from an intensity-angle fit using a rotating analyser and light sensor.

Optical rotation depends not only on the chemical identity of the substance and its concentration, but also on the wavelength of incident light. Literature values are typically reported at the sodium D-line ($\lambda = 589$nm), but many practical systems use different wavelengths. The dispersion of optical rotation with wavelength can be modelled using Drude's equation [2]:

$$[\alpha]^T(\lambda) = \frac{A}{\lambda^2 - \lambda_0^2} \qquad (3)$$

where A and λ_0 are empirically determined constants, and λ_0 represents a characteristic absorption wavelength.
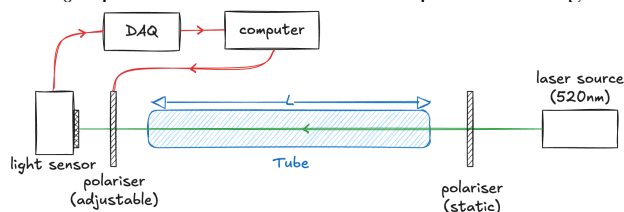
FIG. 1: Experiment setup. A 520 nm laser passes through a static polariser, producing linearly polarised light. The polarisation rotates as it travels through the sample, with the angle measured using an adjustable polariser and a sensor.

This experiment investigates the optical rotation of solutions of sucrose, glucose, and fructose using a green 520 nm laser source. The results are compared against literature values reported at 589 nm, with a dispersion correction applied to reconcile the different wavelengths.

II. Methods

A schematic of the experimental setup is shown in Figure 1. A 520 nm Class 2 laser source was used to generate unpolarised light, which was then passed through a static polariser to produce linearly polarised light. The beam then travelled through a cylindrical tube containing a chiral sample before reaching a computer-controlled adjustable polariser and light sensor. The transmitted intensity was recorded by a DAQ system connected to the sensor and analysed by a computer.

Sucrose, glucose, and fructose solutions were prepared at concentrations ranging from 5 g L^{-1} to 50 g L^{-1}, in 500 mL batches, using distilled water. Each sugar was weighed on a calibrated digital balance and mixed thoroughly to ensure complete dissolution. The tube was cleaned between runs, and dried externally, to prevent contamination and keep the optical interfaces free of moisture or smudges. The tube was filled to capacity to ensure consistent optical path length.

Temperature stability was monitored by periodically checking the temperature of the distilled water used to prepare the solutions. Across all measurement runs, the temperature remained within $\pm 0.5°$C of $20°$C, which was considered negligible.
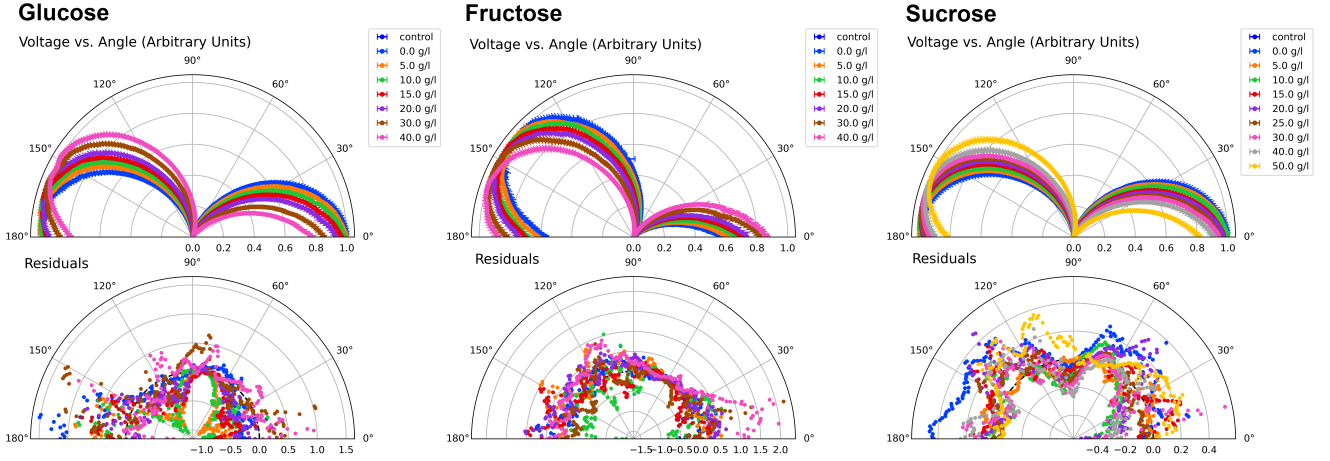
FIG. 2: Polar phase plots of voltage vs. angle for different concentrations of glucose, fructose, and sucrose. The top row shows the measured data, while the bottom row displays the normalized residuals.

A calibration run using pure distilled water was done for each set of measurements to serve as a control, with its measured rotation value subtracted from all subsequent measurements.

For each sample, the adjustable polariser was rotated from $0°$ to $180°$ in $1°$ increments, giving a total of 181 angular steps. At each angle, voltage measurements were acquired over a 0.5 sec interval at a sampling rate of 512 Hz, yielding 256 samples per step. The mean and standard error of these readings were used.

The resulting intensity readings were normalised to a $[0, 1]$ range, allowing Malus' Law to be fit to the form:

$$I = \cos^2(\theta - \phi) \qquad (4)$$

where θ is the polariser angle and ϕ is an adjustable parameter representing the rotation angle. A χ^2 fitting approach was used to determine ϕ, with the extracted optical rotation α for each sample given by $\phi - \phi_0$, where ϕ_0 is the reference rotation from the control measurement. The data showed minimal noise, so no outlier rejection was needed.

Normalisation ensures that the measured intensity falls within a consistent range $[0, 1]$, allowing for direct comparison between different measurements. This was done to account for any variations in sensor sensitivity and ambient light interference during the experiment.

A linear fit of rotation vs. concentration was then applied to extract the specific rotation:

$$\frac{\Delta \alpha}{\Delta c} = [\alpha]_\lambda^T \times l \qquad (5)$$

Thus, the gradient of the optical rotation vs. concentration plot yields the specific rotation

III. Results

We obtained the following values for the specific rotation for sucrose, fructose, and glucose:

Molecule	Measured α (°)	Literature α (°)	χ^2_{reduced}
Sucrose	89.7 ± 1.0	$+67$ [4]	507.49
Fructose	-122.8 ± 1.4	-94 [5]	29.91
Glucose	138.8 ± 1.6	$+52$ [6]	76.14

TABLE I: Measured and literature values for specific rotations.

These values were taken over a single trial for each concentration. The standard errors were taken from the χ^2 fits.

Figure 2 shows that the measured voltage closely follows the expected $\cos^2$ dependence, with minimal noise; however, there are structured deviations in the residual plots. This indicates there may be systematic effects not fully accounted for by the model.

The sucrose measurement at 50 g L^{-1} showed substantial deviation from the expected trend, and was therefore excluded from the concentration-rotation fit.
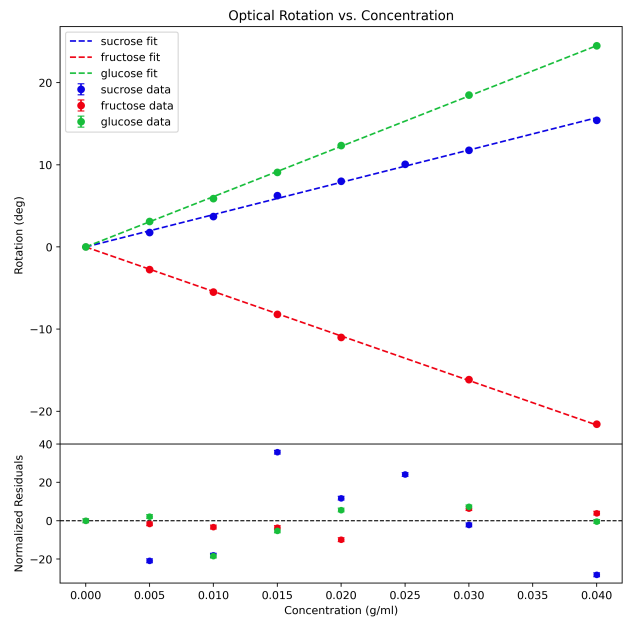
FIG. 3: Optical rotation vs. concentration for sucrose (blue), fructose (red), and glucose (green), with linear fits and residuals shown below.

The quality of the fits to both Malus' law and the concentration-rotation relationships appears visually consistent with expectations. However, the high reduced χ^2 values observed in the concentration-rotation fits suggest that our errors may be underestimated. A likely candidate for this underestimation is the uncertainty in the sample concentrations, which was not explicitly incorporated into the χ^2 calculations. This omission could be contributing to the high χ^2 values and may mask other sources of error.

IV. Discussion

Our measured values for the optical rotation of sucrose, fructose, and glucose deviate considerably from the literature values. In particular, the measured specific rotation for sucrose (approximately $90°$) is notably higher than the literature value of $66.37°$, with similarly large discrepancies observed for fructose and glucose. Although the direction of rotation is correctly determined for all samples, the magnitude of the deviations indicates the presence of systematic errors or unaccounted-for uncertainties in our measurements.

A. Systematic & Measurement Errors

Although uncertainties in sample concentration could contribute to the observed discrepancies, this is unlikely to be the dominant source of error. The fits were highly linear, suggesting the solute masses were measured with sufficient precision. Inaccuracies in mass would more likely manifest as random scatter rather than the consistent global shifts we observe.

One source of error is in precisely measuring the length of the liquid in the tube. For example, the glass interfaces on either side make it hard to correctly estimate the path length. Similarly, if the light travels at a slight angle, this would affect the path length.

Lastly, the patterns observed in the residuals of the angle–intensity plots point toward systematic errors, likely arising from scattered polarized light from the tube. While these hint at the presence of systematic effects, there is no obvious mechanism by which they would lead to the consistent bias seen in the concentration-rotation calibration.

For sucrose, we note that similar measured values ($\sim 90°$) were initially reported by other peers, suggesting that the discrepancy may arise from factors such as sample impurities. In addition, potential errors in the estimation of the effective path length could also contribute to the deviation.

If a single systematic error, such as incorrect path length, was responsible for the deviation from the literature values, we would expect a nearly constant proportionality factor across all molecules. However, instead, we observe measured-to-literature ratios of 1.35, 1.33 and 2.63 across sucrose, fructose, and glucose respectively. This suggests that the source of error is unlikely to be consistent between measurement runs, providing more evidence for the hypotheses that impurities or other sample-specific factors were responsible for these discrepancies.

B. Temperature Effects

The literature values for specific rotation are reported at $20°C$, which matched the ambient temperature during our experiment to within $0.5°C$. Although optical rotation can be temperature-dependent, especially for sugars, the small deviation here makes it unlikely to be a significant factor. Temperature-induced changes in rotation for sucrose are generally small over such narrow ranges, so any resulting shift would be negligible compared to the observed discrepancy.

C. Dispersion Correction

The literature values for specific rotation are typically given at the sodium D-line nm, whereas our experiment used a 520 nm laser. Since optical rotation varies with wavelength due to dispersion, directly comparing our measured values to the literature introduces an inconsistency. To address this, we used the Drude model (3).

Solving A, given λ_0, yields:

$$[\alpha]_D^T = [\alpha]_\lambda^T \frac{\lambda^2 - \lambda_0^2}{\lambda_D^2 - \lambda_0^2} \qquad (6)$$

By applying this to our results, we get:

Molecule	λ_0 (nm)	Measured $[\alpha]_{520}$ (°)	Inferred $[\alpha]_D$ (°)
Sucrose	146 [2]	89.7 ± 1.0	68.6 ± 0.8
Glucose	126.5 [1]	138.8 ± 1.6	106.7 ± 1.2
Fructose	—	-122.8 ± 1.4	—

TABLE II: Drude-model adjusted estimates for specific rotation at 589 nm (sodium D-line), using measured values at 520 nm and literature values for λ_0 where available.

Table II shows the inferred D-line specific rotations for each sample. For sucrose, the corrected value of $68.62 \pm 0.8°$ agrees with the literature value of $66.3°$ [4], suggesting that the discrepancy in the raw measurement might be explained by dispersion. However, the inferred D-line value for glucose remains significantly elevated at $106.7 \pm 1.2°$, nearly double the accepted value of $52.70°$, suggesting the correction is insufficient on its own.

This indicates that additional sources of systematic error, such as impurities or inaccuracies in the effective path length must be contributing. For fructose, no literature value for λ_0 could be found, so no dispersion correction could be applied.

D. Mutarotation in Glucose Solutions

An important chemical phenomenon that may account for the high rotation measured for glucose is mutarotation. When D-glucose is dissolved in water, it exists in an equilibrium mixture of two cyclic stereoisomers: the α and β anomers. These forms interconvert slowly in solution, and each has a distinct specific rotation, approximately $+112°$ for α-glucose and $+19°$ for β-glucose [6].

At room temperature, the equilibrium mixture is a mixture of α- and β- glucose, resulting in an overall specific

rotation of $\sim 52.7°$. However, if a solution is measured shortly after preparation, the α form may still dominate, resulting in an increased specific rotation.

Our dispersion-corrected value for glucose was $+106.7°$, which lies much closer to the α-glucose value than the equilibrium mean. A simple weighted model suggests that a mixture with an approximate 19:1 ratio of α to β anomers would be consistent with this result. This strongly indicates that mutarotation was incomplete at the time of measurement and likely contributed significantly to the observed deviation. It also implies that time-dependent changes in rotation should be expected if glucose solutions are not allowed to equilibrate before measurement.

V. Conclusions

This experiment aimed to investigate optical rotation in chiral sugar solutions, specifically sucrose, glucose, and fructose. By analysing the polarisation of a laser beam after passing through each solution, we extracted rotation angles using Malus' law and determined the corresponding specific rotations.

Our data yielded specific rotation values of approximately $+89.7°$ for sucrose, $+138.8°$ for glucose, and $-122.8°$ for fructose at a wavelength of 520 nm. These values deviate significantly from literature values reported at the sodium D-line (589 nm), which are $+66.37°$, $+52.70°$, and $-92.00°$ respectively.

We applied a dispersion correction using Drude's equation. This adjustment brought the sucrose measurement into agreement with literature ($68.62 \pm 0.77°$), validating both the experimental approach and the necessity of wavelength correction. However, the corrected glucose result ($106.70 \pm 1.23°$) remained anomalously high, and no correction could be applied for fructose due to missing dispersion parameters.

Subsequent analysis revealed that the elevated glucose reading is consistent with mutarotation, a chemical process in which α- and β-glucose interconvert in solution. If the solution is measured shortly after preparation, a large excess of the α anomer (which has a much higher specific rotation) can skew the result. Our corrected glucose value aligns with a mixture of roughly a 19:1 ratio of α- to $beta$-glucose. This suggests that mutarotation had may have not yet reached equilibrium.

The remaining discrepancies likely arise from sources such as inaccurate path length estimation or sample impurities. The fact that deviations varied significantly between molecules supports the view that dominant errors were measurement-specific.

Despite these limitations, the experiment succeeded in identifying the correct direction of rotation for each sample, and confirmed the expected linear relationship between concentration and optical rotation.

Limitations of the experiment include the use of only a single trial per concentration, which prevented analysis of repeatability or statistical variance. In addition, the uncertainty in the concentrations was not propagated into the error model, likely contributing to the high reduced χ^2 values observed in the concentration–rotation fits.

Future experiments could improve on these limitations by employing multiple trials, verified-purity samples, and more precisely measured optical path lengths (e.g., using cuvettes). Allowing sufficient time for mutarotation to complete prior to measurement would also reduce chemical variability, particularly for glucose. Finally, measuring optical rotation at several different wavelengths would allow direct observation of dispersion curves and potentially enable independent estimation of Drude model parameters.

Ultimately, while absolute values deviated from literature, the experiment successfully captured the qualitative behaviour of optical rotation, and may have directly observed the effects of mutarotation.

References

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Appendix A: Error Appendix

1. Measurement Uncertainties

The optical path length of the sample tube was measured with a ruler. The uncertainty was taken as ± 0.1cm, accounting for both parallax and calibration error. This value was treated as a single absolute uncertainty and entered directly into the error propagation for specific rotation. No separate end-to-end propagation was applied due to the use of a single fixed measurement.

The photodiode voltage was sampled at a rate of 512 Hz over a 0.5 s interval at each polariser angle, giving $N = 256$ samples per angle. The mean voltage $\bar{V}$ and its standard error α_V were calculated as:

$$\bar{V} = \frac{1}{N} \sum_{i=1}^{N} V_i \qquad (7)$$

$$\sigma_{\text{sample}} = \sqrt{\frac{1}{N-1} \sum_{i=1}^{N} (V_i - \bar{V})^2} \qquad (8)$$

$$\alpha_V = \frac{\sigma_{\text{sample}}}{\sqrt{N}} \qquad (9)$$

This standard error was used as the per-point uncertainty in the angle–intensity fits to Malus' law.

2. χ^2-Minimisation for Parameter Fitting

Rotation angles ϕ were extracted by fitting the measured voltages to the function $I(\theta) = \cos^2(\theta + \phi)$, using non-linear least squares minimisation. The fit statistic used was:

$$\chi^2 = \sum_i \left(\frac{V_i - I(\theta_i; \phi)}{\alpha_{V,i}} \right)^2 \qquad (10)$$

To account for possible model mismatch or underestimation of noise, the resulting uncertainties in ϕ were scaled by the square root of the reduced χ^2, given by:

$$\chi^2_{\text{red}} = \frac{\chi^2}{\nu} \qquad (11)$$

where ν is the number of degrees of freedom in the fit.

3. Error Propagation for Specific Rotation

The specific rotation was obtained from the slope m of the linear fit between rotation angle and concentration, using the relation:

$$[\alpha] = \frac{m}{l} \qquad (12)$$

The uncertainty in $[\alpha]$ was calculated via:

$$\sigma_{[\alpha]} = [\alpha] \cdot \sqrt{\left(\frac{\sigma_m}{m} \right)^2 + \left(\frac{\sigma_l}{l} \right)^2} \qquad (13)$$

where σ_m is the uncertainty in the fitted slope and σ_l is the uncertainty in the optical path length.

Each measured rotation α was calculated relative to a control (distilled water) measurement, ϕ_0. The associated uncertainty was computed in quadrature:

$$\sigma_\alpha = \sqrt{\sigma_\phi^2 + \sigma_{\phi_0}^2} \qquad (14)$$

4. Drude Dispersion Correction

To account for wavelength-dependent dispersion of optical rotation, corrected values at the sodium D-line (589nm) were calculated using Drude's model:

$$[\alpha](\lambda) = \frac{A}{\lambda^2 - \lambda_0^2} \qquad (15)$$

Given a measured $[\alpha]_\lambda$ at $\lambda = 520$nm, the constant A was inferred via:

$$A = [\alpha]_\lambda \cdot (\lambda^2 - \lambda_0^2) \qquad (16)$$

with uncertainty propagated as:

$$\sigma_A = \sigma_{[\alpha]_\lambda} \cdot (\lambda^2 - \lambda_0^2) \qquad (17)$$

The corrected value $[\alpha]_D$ at 589nm was then calculated as:

$$[\alpha]_D = \frac{A}{\lambda_D^2 - \lambda_0^2} \qquad (18)$$

with uncertainty:

$$\sigma_{[\alpha]_D} = \frac{\sigma_A}{\lambda_D^2 - \lambda_0^2} \qquad (19)$$

This method assumes negligible uncertainty in λ_0, which was taken from literature values. Corrections could not be applied for substances lacking known λ_0.

Scientific Summary for a General Audience

This experiment explored how certain sugars (sucrose, glucose, and fructose) interact with light. Specifically, it measured a property called optical rotation, where molecules twist the orientation of polarised light as it passes through them. This effect is common in "chiral" molecules, which are asymmetrical and have mirror-image forms.

Using a laser and a sensor setup, we passed light through sugar solutions and measured how much the light's orientation rotated. These measurements can help identify substances or check their purity, something commonly done in chemistry and food science.

We found that while the direction of rotation (clockwise or anticlockwise) matched expectations, the strength of the rotation was often much higher than expected. After correcting for differences in laser wavelength and analysing possible sources of error, we concluded that some deviations likely came from the chemistry of the sugars themselves. In particular, glucose undergoes a process called mutarotation when dissolved, gradually shifting its molecular form in a way that affects the result.

Overall, the experiment confirmed the basic physics of optical rotation and showed how both physical setup and chemical behaviour influence the results. It also highlighted how subtle changes, such as measuring too soon, can meaningfully affect outcomes in scientific experiments.

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