



INSTITUTE FOR ENGINEERING THERMODYNAMICS  
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Laboratory course report  
**Application of Raman spectroscopy**

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# Todo list

[MK1]: Error discussion Temp missing . . . . . 6

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# 1 Introduction

Some fancy introduction.

The assignment, description of the equipment and procedure and further details about the Lab Course are described in the given handbook [1].

## **2 Theoretical basics**

The following theoretical basics are summarized from the standard literature in optics [2]–[5] and more specifically Raman application [6], [7].

### **2.1 Molecule - light interactions**

### **2.2 Scattering effects**

### **2.3 Measurement of different physical properties - RAMAN spectroscopy**

## **3 Experimental setup**

### **3.1 Used equipment**

### **3.2 Measurement setup and preparations**

### **3.3 Expectations**

### **3.4 Execution**



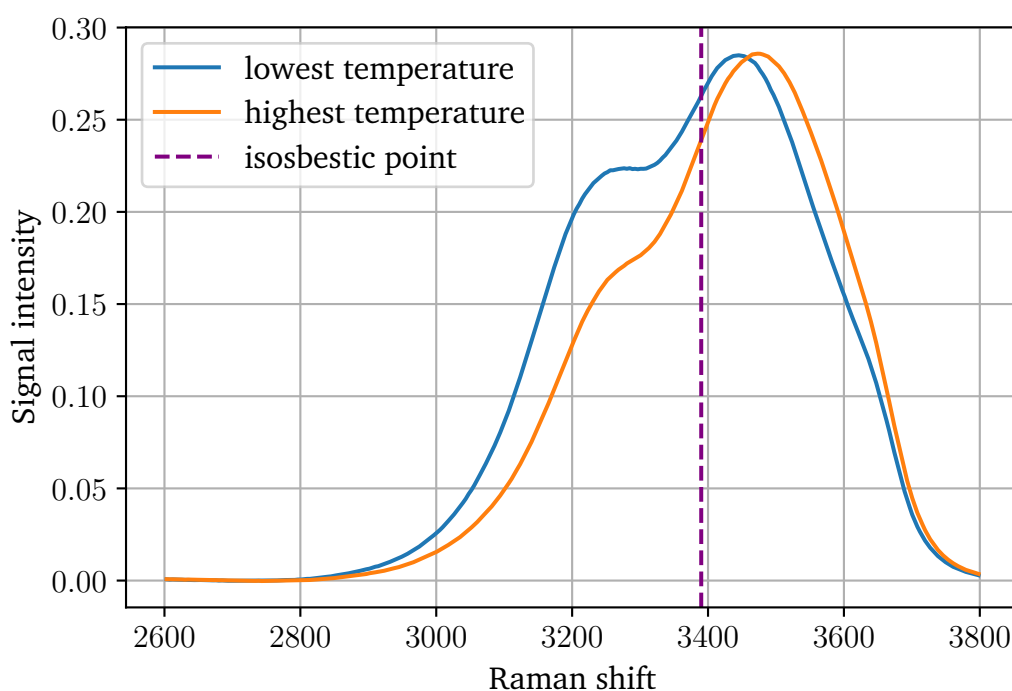
# 4 Results

## 4.1 Data presentation and preparation

### Species determination

### Temperature calculation

The raw data of the intensity spectrum over the Raman shift can be obtained in Figure 4.1.



**Figure 4.1:** Plot of the absolute scattering intensities over the Raman shift  $\Delta\tilde{\nu}$ ; Plot at the highest recorded temperature and the lowest recorded temperature for simplification purposes

## 4.2 Evaluation and error discussion

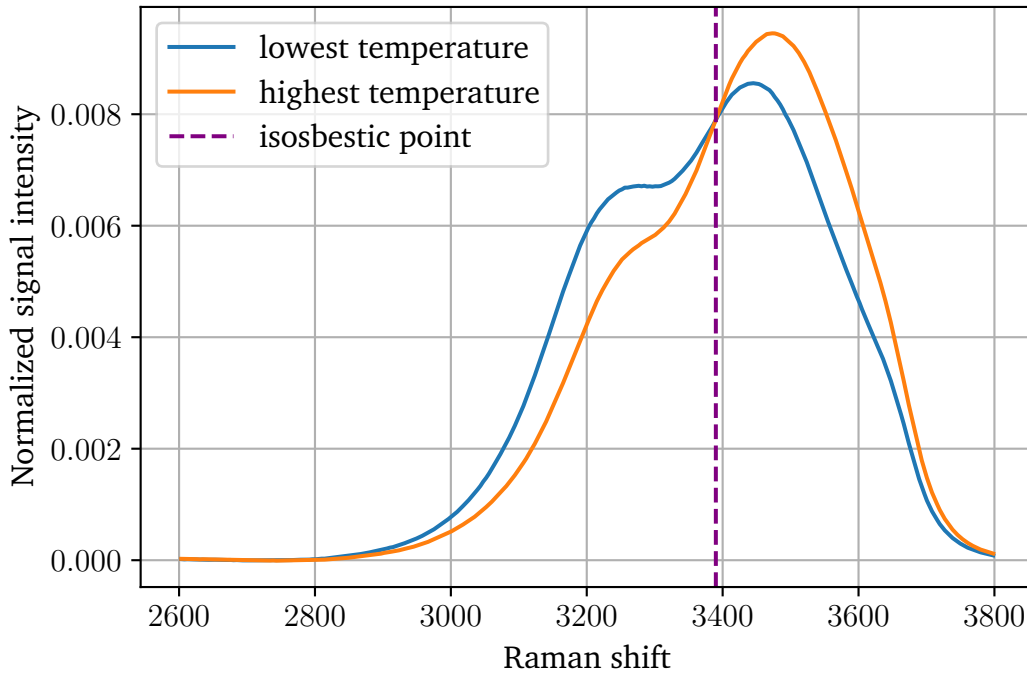
### Species determination

Text and data from JP.

Plots need to be integrated.

## Temperature calculation

The plot of the change of scattered intensities over the Raman shift is illustrated in Figure 4.2. The isosbestic point can be determined at roughly  $3390\text{cm}^{-1}$ , via the lowest standard deviation of all the normalized data sets. The areas can be interpreted as the integration of the curve within the boundaries  $[3390\text{ cm}^{-1}, 3800\text{ cm}^{-1}]$  for  $A_{\text{right}}$ , and  $[2600\text{ cm}^{-1}, 3390\text{ cm}^{-1}]$  for  $A_{\text{left}}$ . Due to the already integrating behavior of the CCD sensor, it is calculated as the sum of all data points within the presented ranges.



**Figure 4.2:** Plot of the area-normalized scattering intensities over the Raman shift  $\Delta\tilde{\nu}$ ; Plot at the highest recorded temperature and the lowest recorded temperature for simplification purposes

With the record of a temperature calibration curve, a function with the form

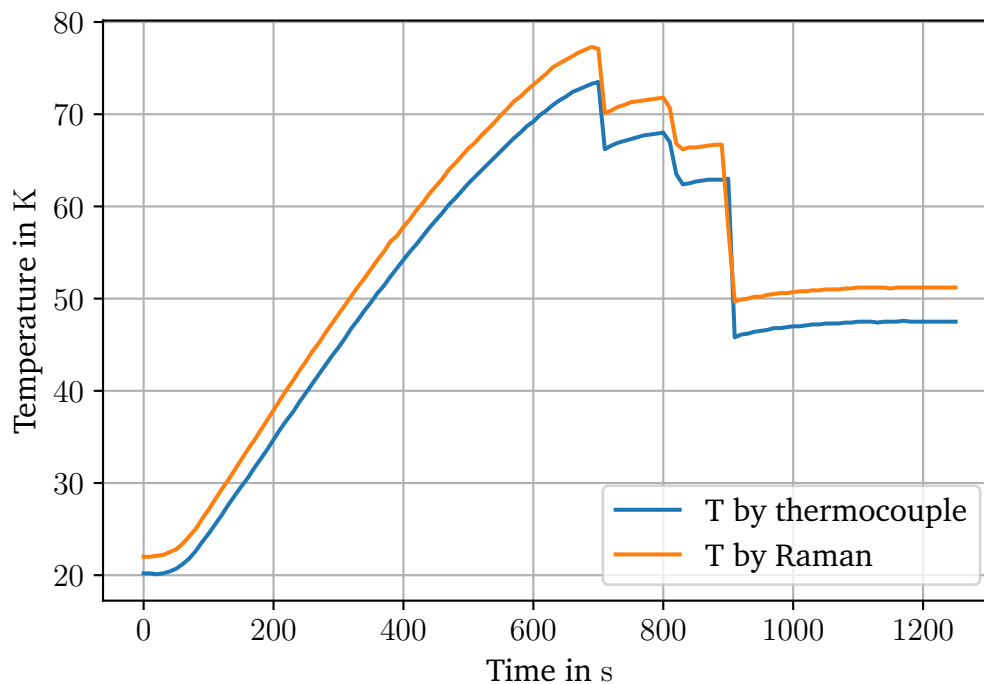
$$T(x) = 42.1 \cdot x^3 - 200.5 \cdot x^2 + 412.4 \cdot x - 233.7 \quad (4.1)$$

can be fitted to calculate the temperature of the liquid through putting in the area ratios  $x$ . The in between results and the final temperature for the highest and the lowest temperature curve are shown in Table 4.1. Compared to the measurement with the

thermocouple K, there is a mean error of 3.46 K, and a mean squared error of 12.83 K over all measurements.

**Table 4.1:** Calculation results for temperature determination through Raman spectroscopy; comparing with the temperature value of the thermocouple K; only for the highest and the lowest temperature due to simplification

	highest temperature	lowest temperature
area ratio	1.51281	1.01273
determined T Raman	77.08 K	22.04 K
measured T thermocouple	73.5 K	20.2 K
error	3.58 K	1.84 K



**Figure 4.3:** Temperature comparison between measurement with the Thermocouple type K and through the Raman setup; plot of temperature over the measurement time

[MK1]: Error  
discussion  
Temp missing

## 5 Summary



# Bibliography

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- [4] S. G. Lipson, H. S. Lipson, and D. S. Tannhauser, *Optik*. Berlin, Heidelberg: Springer Berlin Heidelberg : Imprint : Springer, 1997, ISBN: 978-3-642-59053-5.
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