INSTITUTE FOR ENGINEERING THERMODYNAMICS
Chairman: Prof. Dr.-Ing. Stefan Will

Laboratory course report

Optical Diagnostics in Energy and Process Engineering - Application of Raman spectroscopy

Authors: Maximilian Köhler (23176975)
Energy technology (Master)

Jean-Pascal Lafleur (Mat. Nr.)
Mechanical engineering (Master)

Supervisor: M.Sc. Philipp Bräuer

Group: 2

Execution date: January 23, 2024

Submission date: February 07, 2024

[January 31, 2024 at 22:39 – preliminary version 0.1]

Todo list

[MK1]: Error discussion Temp missing 6

Contents

List of Figures III

List of Tables IV

1 Introduction 1

2 Theoretical basics 2
- 2.1 Molecule - light interactions . . . 2
- 2.2 Scattering effects . . . 2
- 2.3 Measurement of different phisical properties - RAMAN spectroscopy . . . 2

3 Experimental setup 3
- 3.1 Used equipment . . . 3
- 3.2 Measurement setup and preparations . . . 3
- 3.3 Expectations . . . 3
- 3.4 Execution . . . 3

4 Results 4
- 4.1 Data presentation and preparation . . . 4
- 4.2 Evaluation and error discussion . . . 4

5 Summary 7

Bibliography V

List of Figures

4.1 Absolute Raman shift intensities for the lowest and highest temperatures 4
4.2 Area-normalized Raman shift intensities for the lowest and highest temperatures 5
4.3 Temperature comparison between Thermocouple and Raman measurement 6

List of Tables

4.1 Temperature calculation results comparison 6

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 phisical 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 intesity spectrum over the Raman shift can be obtained in Figure 4.1.

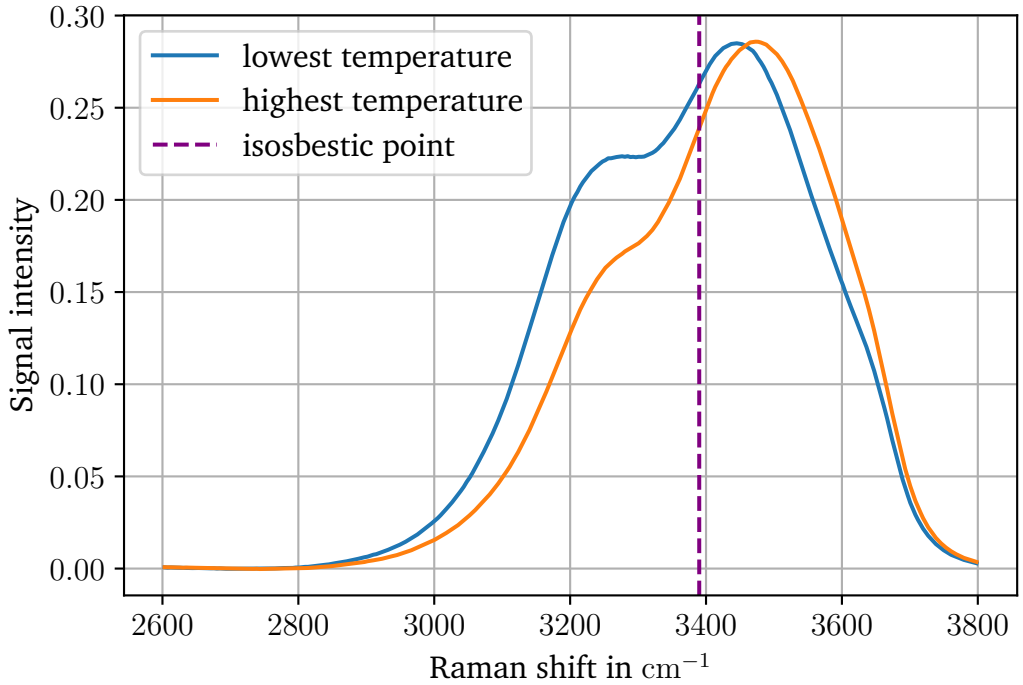

Figure 4.1: Plot of the absolute scattering intensities over the Raman shift $\Delta\tilde{\nu}$; Plot at the highest recorded temperature and the lowest recorded temperature for simplification purposes

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 3390cm^{-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_{right}, and $[2600\ \text{cm}^{-1},\ 3390\ \text{cm}^{-1}]$ for A_{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.

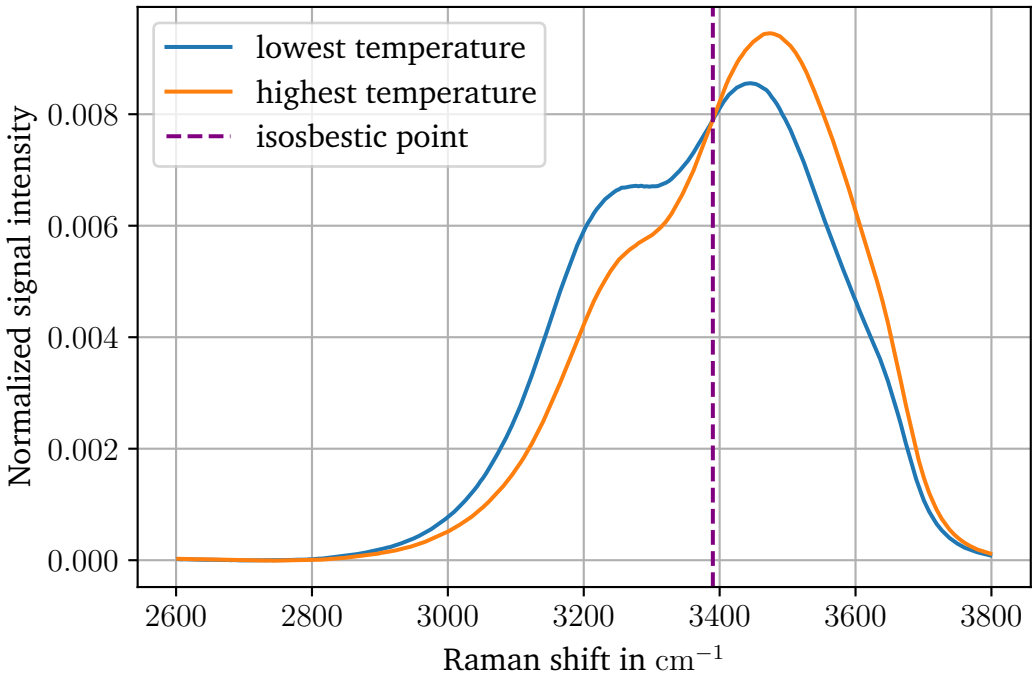

Figure 4.2: Plot of the area-normalized scattering intensities over the Raman shift $\Delta\tilde{\nu}$; Plot at the highest recorded temperature and the lowest recorded temperature for simplification purposes

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

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

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

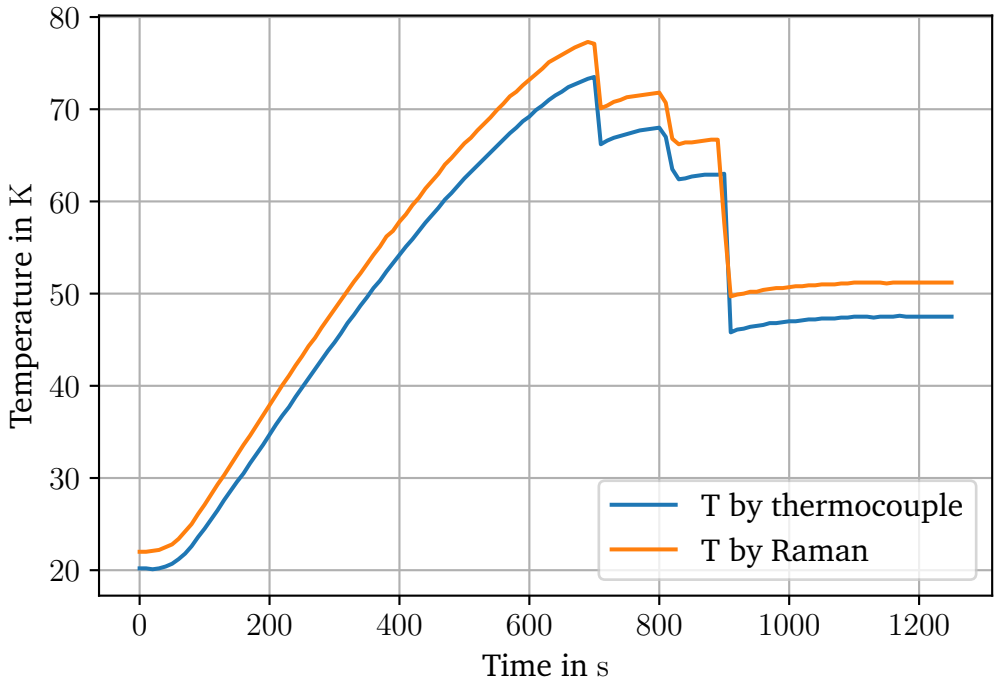

Figure 4.3: Temperature comparison between measurement with the Thermocouple type K and through the Raman setup; plot of temperature over the measurement time

[MK1]: Error discussion Temp missing

5 Summary

Bibliography

[1] P. Bräuer, *Application of Raman spectroscopy*, Winter term 2022/2023.

[2] M. Born and E. Wolf, *Principles of Optics: Electromagnetic Theory of Propagation, Interference and Diffraction of Light*, 7th expanded ed. Cambridge ; New York: Cambridge University Press, 1999, 952 pp., ISBN: 978-0-521-64222-4 978-0-521-63921-7.

[3] E. Hecht and E. Hecht, *Optik*, 4., überarb. Aufl. München Wien: Oldenbourg, 2005, 1116 pp., ISBN: 978-3-486-27359-5.

[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.

[5] H. Niedrig, Ed., *Optik: Wellen- und Teilchenoptik: Part 1* (Lehrbuch der Experimentalphysik / Bergmann; Schaefer 3, Part 1), 10. Auflage[Ausg. in 8 Bänden]. Berlin: de Gruyter, 2004, 668 pp., ISBN: 978-3-11-017081-8.

[6] Herzberg and Huber, *Molecular Spectra and Molecular Structure. 4, Constants of Diatomic Molecules*, Ristampa anastatica. Berlin: Springer, 2013, ISBN: 978-1-4757-0963-6.

[7] B. Schrader and D. Bougeard, *Infrared and Raman Spectroscopy: Methods and Applications*. Weinheim: VCH, 1995, ISBN: 978-3-527-61543-8.