

IR + Raman - IR- and Raman-Spectroscopy

Protocol for the PC 2 lab course by
Vincent Kümmerle & Elvis Gnaglo & Julian Brügger

University of Stuttgart

authors: Vincent Kümmerle, 3712667
st187541@stud.uni-stuttgart.de

Elvis Gnaglo, 3710504
st189318@stud.uni-stuttgart.de

Julian Brügger, 3715444
st190050@stud.uni-stuttgart.de

group number: A05

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supervisor: Mansha Shafquath

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Abstract:

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1 Theory

[1]

2 Procedure

To simulate and calculate the vibrational normal modes, the program `Avogadro2` was used. The structures of the molecules methane, chloromethane, dichloromethane, dibromomethane, chloroform, deuterated chloroform, tetrachloromethane and tetrachloroethylene were built, their geometry was optimized and the optimized coordinates were used to calculate the vibrational modes with the `ORCA` software, resulting in a list of IR and Raman frequencies and intensities for each molecule.

In the experimental part, the Raman spectra of dichloromethane, dibromomethane, chloroform, deuterated chloroform, tetrachloromethane and tetrachloroethylene were measured and analyzed with the `WPenlighten` software. The IR spectra of dichloromethane, dibromomethane, chloroform and tetrachloroethylene were measured using an ATR spectrometer and analyzed with the `Opus` software.

3 Results and Analysis

3.1 Methane

3.1.1 IR

Tab. 1: Listed are the calculated wavenumbers and intensities of the IR signals of CH_4 with the corresponding type of the vibrational mode.

| signal | wavenumber $\tilde{\nu}$ / cm^{-1} | intensity / $\text{KM}\cdot\text{mol}^{-1}$ | vibration type |
|--------|---|---|------------------|
| 1 | 1313.45 | 13.30 | asym. bending |
| 2 | 1313.68 | 13.25 | asym. bending |
| 3 | 1313.73 | 13.25 | asym. bending |
| 4 | 1530.79 | 0 | sym. bending |
| 5 | 1531.05 | 0 | sym. bending |
| 6 | 3019.38 | 0 | sym. stretching |
| 7 | 3152.03 | 17.69 | asym. stretching |
| 8 | 3152.33 | 17.64 | asym. stretching |
| 9 | 3152.45 | 17.64 | asym. stretching |

3.1.2 Raman

Tab. 2: Listed are the calculated wavenumbers and intensities of the Raman signals of CH₄ with the corresponding type of the vibrational mode.

| signal | wavenumber $\tilde{\nu}$ / cm ⁻¹ | Raman intensity / Å ⁴ · amu ⁻¹ | vibration type |
|--------|---|--|------------------|
| 1 | 1313.38 | 1.64419 | asym. bending |
| 2 | 1313.61 | 1.6422 | asym. bending |
| 3 | 1314.1 | 1.6484 | asym. bending |
| 4 | 1531.00 | 27.4565 | sym. bending |
| 5 | 1531.09 | 27.449 | sym. bending |
| 6 | 3019.41 | 145.177 | sym. stretching |
| 7 | 3150.24 | 62.8181 | asym. stretching |
| 8 | 3150.27 | 62.8724 | asym. stretching |
| 9 | 3150.79 | 62.8305 | asym. stretching |

3.2 Chloromethane

3.2.1 IR

3.2.2 Raman

3.3 Dichloromethane

3.3.1 IR

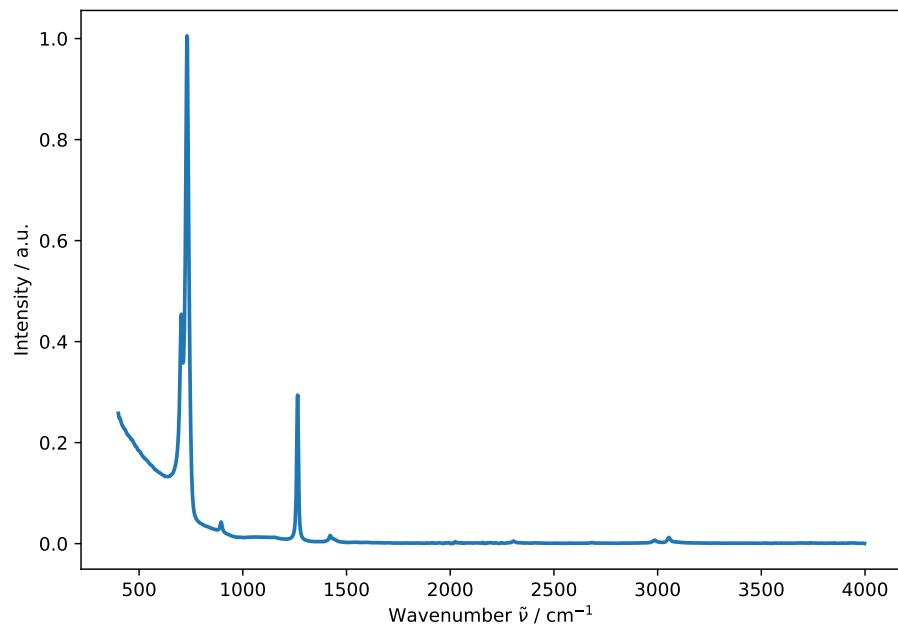


Fig. 1: Measured IR spectrum of dichloromethane.

Tab. 3: Listed are the measured wavenumbers and intensities of the IR signals of CH_2Cl_2 .

| signal | wavenumber $\tilde{\nu}$ / cm $^{-1}$ | intensity / a.u. |
|--------|---------------------------------------|------------------|
| 1 | 704.00 | 0.45 |
| 2 | 730.53 | 1.01 |
| 3 | 895.82 | 0.04 |
| 4 | 1265.17 | 0.29 |
| 5 | 1422.29 | 0.02 |

Tab. 4: Listed are the simulated wavenumbers and intensities of the vibrational modes of CH_2Cl_2 .

| Mode | Wavenumber $\tilde{\nu}$ / cm^{-1} | Intensity / km mol^{-1} |
|------|---|----------------------------------|
| 1 | 277.23 | 0.64 |
| 2 | 703.86 | 14.19 |
| 3 | 733.80 | 137.83 |
| 4 | 889.17 | 1.20 |
| 5 | 1153.54 | 0.00 |
| 6 | 1272.86 | 41.21 |
| 7 | 1441.46 | 0.01 |
| 8 | 3107.43 | 9.81 |
| 9 | 3194.30 | 0.64 |

3.3.2 Raman

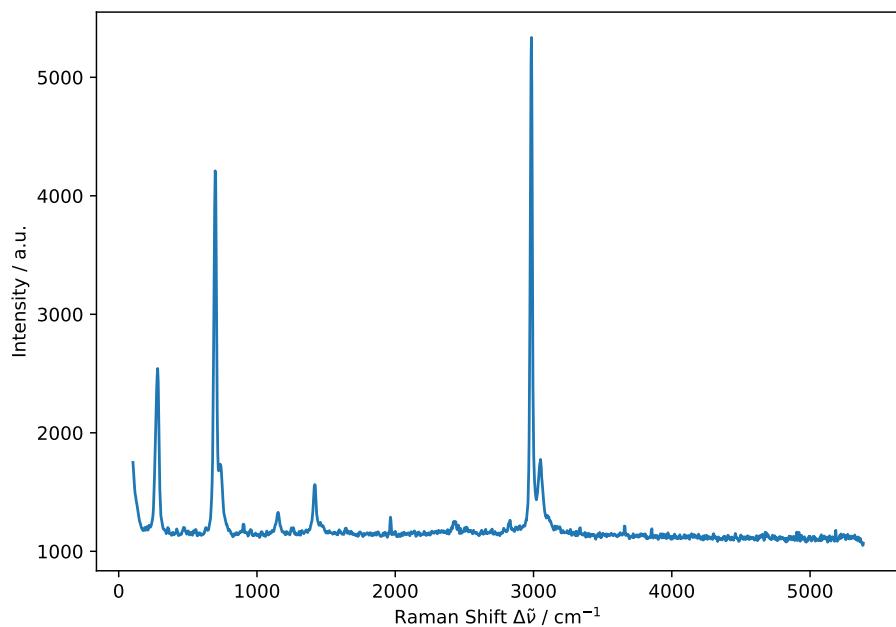


Fig. 2: Measured raman spectrum of dichloromethane.

Tab. 5: Listed are the measured Raman shifts and intensities of the signals of CH_2Cl_2 .

| signal | Raman Shift $\Delta\tilde{\nu}$ / cm^{-1} | intensity / a.u. |
|--------|--|------------------|
| 1 | 281.99 | 2542.67 |
| 2 | 697.77 | 4210.67 |
| 3 | 1418.07 | 1563.33 |
| 4 | 2984.85 | 5336.00 |
| 5 | 3051.13 | 1775.33 |

Tab. 6: Listed are the simulated wavenumbers and raman intensities of the vibrational modes of CH_2Cl_2 .

| Mode | Wavenumber $\tilde{\nu}$ / cm^{-1} | Raman Intensity / $\text{\AA}^4 \text{amu}^{-1}$ |
|------|---|--|
| 1 | 277.06 | 6.83 |
| 2 | 703.48 | 12.27 |
| 3 | 732.67 | 5.02 |
| 4 | 888.90 | 3.13 |
| 5 | 1153.83 | 11.78 |
| 6 | 1272.67 | 3.01 |
| 7 | 1441.64 | 12.42 |
| 8 | 3106.65 | 108.70 |
| 9 | 3193.09 | 62.65 |

3.4 Dibromomethane

3.4.1 IR

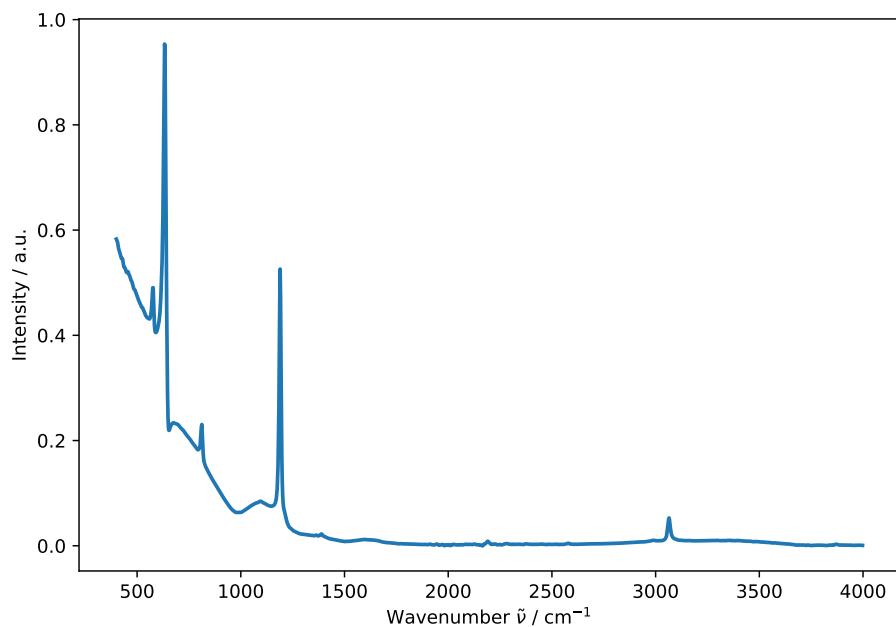


Fig. 3: Measured IR spectrum of dibromomethane.

Tab. 7: Listed are the measured wavenumbers and intensities of the IR signals of CH_2Br_2 .

| signal | wavenumber $\tilde{\nu}$ / cm^{-1} | intensity / a.u. |
|--------|---|------------------|
| 1 | 455.05 | 0.52 |
| 2 | 577.49 | 0.49 |
| 3 | 632.58 | 0.95 |
| 4 | 677.48 | 0.23 |
| 5 | 812.16 | 0.23 |
| 6 | 1095.80 | 0.08 |
| 7 | 1189.66 | 0.53 |
| 8 | 1389.64 | 0.02 |
| 11 | 3064.97 | 0.05 |

Tab. 8: Listed are the simulated wavenumbers and intensities of the vibrational modes of CH_2Br_2 .

| Mode | Wavenumber $\tilde{\nu}$ / cm^{-1} | Intensity / km mol^{-1} |
|------|---|----------------------------------|
| 1 | 168.72 | 0.08 |
| 2 | 573.58 | 4.08 |
| 3 | 628.31 | 98.95 |
| 4 | 806.07 | 4.64 |
| 5 | 1101.92 | 0.00 |
| 6 | 1205.80 | 65.32 |
| 7 | 1412.95 | 0.00 |
| 8 | 3126.16 | 1.92 |
| 9 | 3221.84 | 1.28 |

3.4.2 Raman

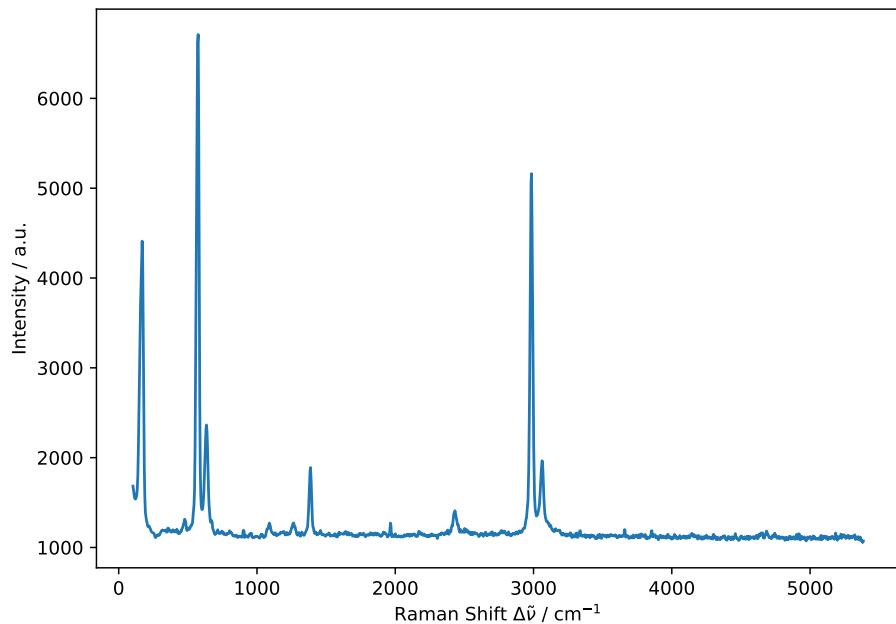


Fig. 4: Measured raman spectrum of dibromomethane.

Tab. 9: Listed are the measured Raman shifts and intensities of the signals of CH_2Br_2 .

| signal | Raman Shift $\Delta\tilde{\nu}$ / cm $^{-1}$ | intensity / a.u. |
|--------|--|------------------|
| 1 | 169.61 | 4410.67 |
| 2 | 574.79 | 6711.00 |
| 3 | 634.60 | 2364.33 |
| 4 | 1387.16 | 1889.33 |
| 5 | 2432.07 | 1409.00 |
| 6 | 2984.85 | 5162.00 |
| 7 | 3062.11 | 1965.67 |

Tab. 10: Listed are the simulated wavenumbers and raman intensities of the vibrational modes of CH_2Br_2 .

| Mode | Wavenumber $\tilde{\nu}$ / cm^{-1} | Raman Intensity / $\text{\AA}^4 \text{ amu}^{-1}$ |
|------|---|---|
| 1 | 168.56 | 5.37 |
| 2 | 574.64 | 13.43 |
| 3 | 629.71 | 5.36 |
| 4 | 806.60 | 2.41 |
| 5 | 1102.17 | 8.43 |
| 6 | 1205.71 | 0.74 |
| 7 | 1413.22 | 13.77 |
| 8 | 3125.63 | 97.24 |
| 9 | 3221.31 | 58.05 |

3.5 Chloroform

3.5.1 IR

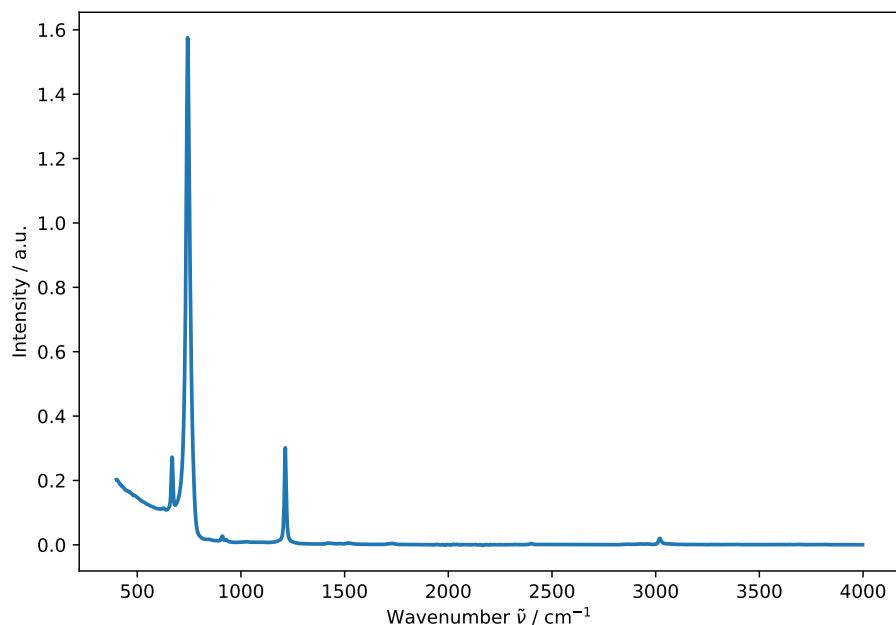


Fig. 5: Measured IR spectrum of chloroform.

Tab. 11: Listed are the measured wavenumbers and intensities of the IR signals of CHCl₃.

| signal | wavenumber $\tilde{\nu}$ / cm ⁻¹ | intensity / a.u. |
|--------|---|------------------|
| 1 | 626.46 | 0.11 |
| 2 | 667.27 | 0.27 |
| 3 | 742.78 | 1.58 |
| 4 | 910.10 | 0.03 |
| 5 | 928.47 | 0.02 |
| 6 | 1214.15 | 0.30 |
| 7 | 3020.07 | 0.02 |

Tab. 12: Listed are the simulated wavenumbers and intensities of the vibrational modes of CHCl₃.

| Mode | Wavenumber $\tilde{\nu}$ / cm ⁻¹ | Intensity / km mol ⁻¹ |
|------|---|----------------------------------|
| 1 | 254.78 | 0.06 |
| 2 | 254.97 | 0.06 |
| 3 | 362.33 | 0.46 |
| 4 | 665.85 | 7.26 |
| 5 | 741.92 | 167.74 |
| 6 | 742.13 | 167.67 |
| 7 | 1220.08 | 22.80 |
| 8 | 1220.17 | 22.76 |
| 9 | 3169.43 | 0.22 |

3.5.2 Raman

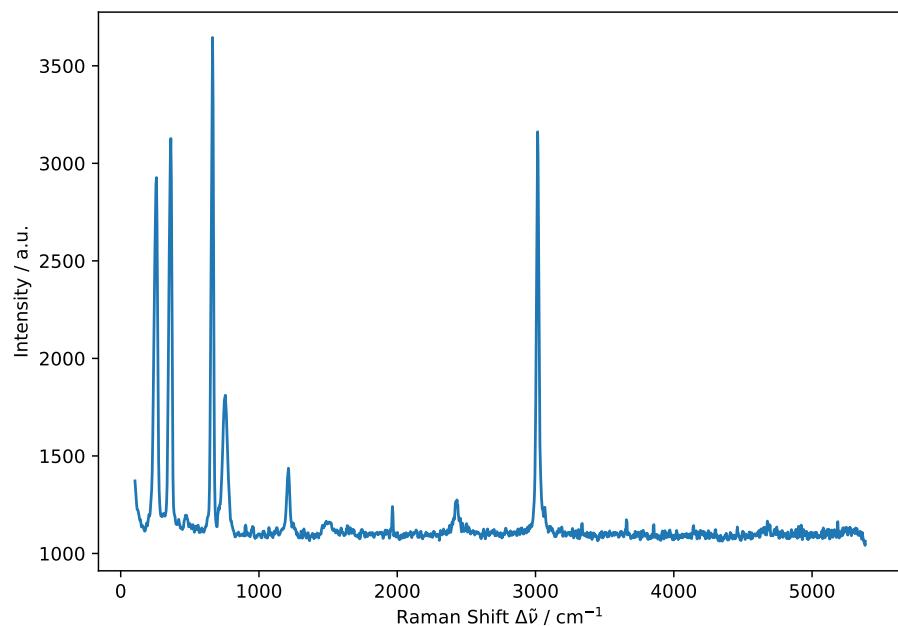


Fig. 6: Measured raman spectrum of chloroform.

Tab. 13: Listed are the measured Raman shifts and intensities of the signals of CHCl₃.

| signal | Raman Shift $\Delta\tilde{\nu}$ / cm $^{-1}$ | intensity / a.u. |
|--------|--|------------------|
| 1 | 258.84 | 2927.00 |
| 2 | 362.65 | 3127.33 |
| 3 | 664.38 | 3645.00 |
| 4 | 756.86 | 1811.33 |
| 5 | 1213.44 | 1437.33 |
| 6 | 3015.32 | 3161.67 |

Tab. 14: Listed are the simulated wavenumbers and raman intensities of the vibrational modes of CHCl_3 .

| Mode | Wavenumber $\tilde{\nu}$ / cm^{-1} | Raman Intensity / $\text{\AA}^4 \text{ amu}^{-1}$ |
|------|---|---|
| 1 | 254.60 | 5.14 |
| 2 | 255.07 | 5.13 |
| 3 | 362.22 | 8.69 |
| 4 | 665.69 | 9.80 |
| 5 | 740.88 | 3.08 |
| 6 | 741.45 | 3.07 |
| 7 | 1220.22 | 6.04 |
| 8 | 1220.68 | 6.05 |
| 9 | 3168.77 | 77.28 |

3.6 Deuterated Chloroform

3.6.1 IR

Tab. 15: Listed are the simulated wavenumbers and intensities of the vibrational modes of CDCl_3 .

| Mode | Wavenumber $\tilde{\nu}$ / cm^{-1} | Intensity / km mol^{-1} |
|------|---|----------------------------------|
| 1 | 253.69 | 0.06 |
| 2 | 253.88 | 0.06 |
| 3 | 360.12 | 0.50 |
| 4 | 646.14 | 6.66 |
| 5 | 717.83 | 125.46 |
| 6 | 717.98 | 125.28 |
| 7 | 909.65 | 63.16 |
| 8 | 909.66 | 63.19 |
| 9 | 2342.61 | 0.74 |

3.6.2 Raman

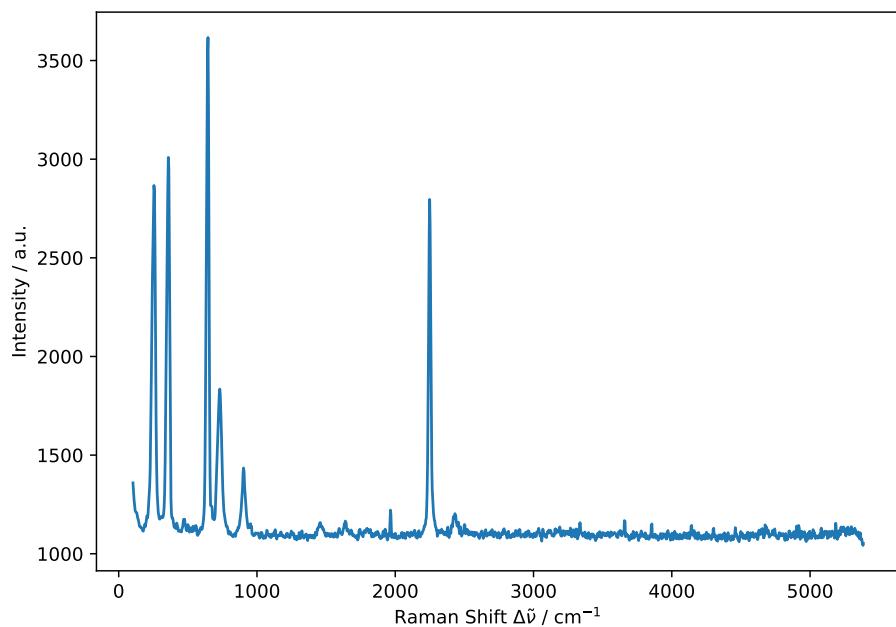


Fig. 7: Measured raman spectrum of deuterated chloroform.

Tab. 16: Listed are the measured Raman shifts and intensities of the signals of CDCl_3 .

| signal | Raman Shift $\Delta\tilde{\nu}$ / cm $^{-1}$ | intensity / a.u. |
|--------|--|------------------|
| 1 | 254.97 | 2866.67 |
| 2 | 358.83 | 3009.00 |
| 3 | 645.78 | 3616.67 |
| 4 | 731.05 | 1834.67 |
| 5 | 903.05 | 1434.67 |
| 6 | 2248.93 | 2796.00 |

Tab. 17: Listed are the simulated wavenumbers and raman intensities of the vibrational modes of CDCl_3 .

| Mode | Wavenumber $\tilde{\nu}$ / cm^{-1} | Raman Intensity / $\text{\AA}^4 \text{ amu}^{-1}$ |
|------|---|---|
| 1 | 254.60 | 5.14 |
| 2 | 255.07 | 5.13 |
| 3 | 362.22 | 8.69 |
| 4 | 665.69 | 9.80 |
| 5 | 740.88 | 3.08 |
| 6 | 741.45 | 3.07 |
| 7 | 1220.22 | 6.04 |
| 8 | 1220.68 | 6.05 |
| 9 | 3168.77 | 77.28 |

3.7 Tetrachloromethane

3.7.1 IR

Tab. 18: Listed are the simulated wavenumbers and intensities of the vibrational modes of CCl_4 .

| Mode | Wavenumber $\tilde{\nu}$ / cm^{-1} | Intensity / km mol^{-1} |
|------|---|----------------------------------|
| 1 | 212.71 | 0.00 |
| 2 | 212.89 | 0.00 |
| 3 | 310.72 | 0.06 |
| 4 | 310.82 | 0.06 |
| 5 | 310.88 | 0.06 |
| 6 | 451.20 | 0.00 |
| 7 | 754.80 | 185.52 |
| 8 | 755.02 | 185.61 |
| 9 | 755.51 | 185.58 |

3.7.2 Raman

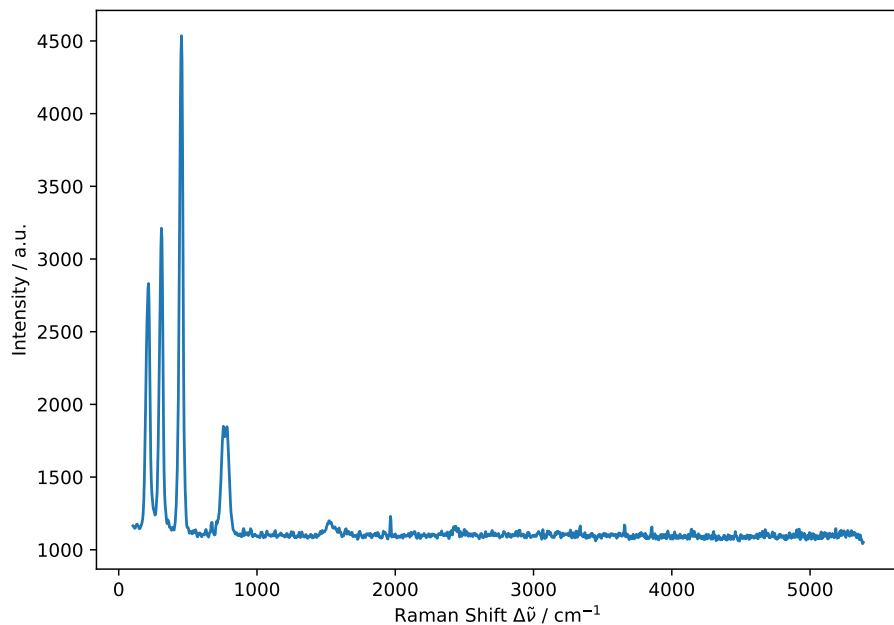


Fig. 8: Measured raman spectrum of tetrachloromethane.

Tab. 19: Listed are the measured Raman shifts and intensities of the signals of CCl_4 .

| signal | Raman Shift $\Delta\tilde{\nu}$ / cm^{-1} | intensity / a.u. |
|--------|--|------------------|
| 1 | 216.25 | 2831.33 |
| 2 | 308.95 | 3211.67 |
| 3 | 454.10 | 4535.33 |
| 4 | 756.86 | 1849.33 |

Tab. 20: Listed are the simulated wavenumbers and Raman intensities of the vibrational modes of CCl_4 .

| Mode | Wavenumber $\tilde{\nu}$ / cm^{-1} | Raman Intensity / $\text{\AA}^4 \text{ amu}^{-1}$ |
|------|---|---|
| 1 | 212.71 | 4.18 |
| 2 | 212.91 | 4.17 |
| 3 | 310.52 | 5.39 |
| 4 | 310.84 | 5.40 |
| 5 | 311.16 | 5.40 |
| 6 | 451.08 | 16.40 |
| 7 | 753.44 | 1.55 |
| 8 | 754.26 | 1.56 |
| 9 | 754.60 | 1.54 |

3.8 Tetrachloroethylene

3.8.1 IR

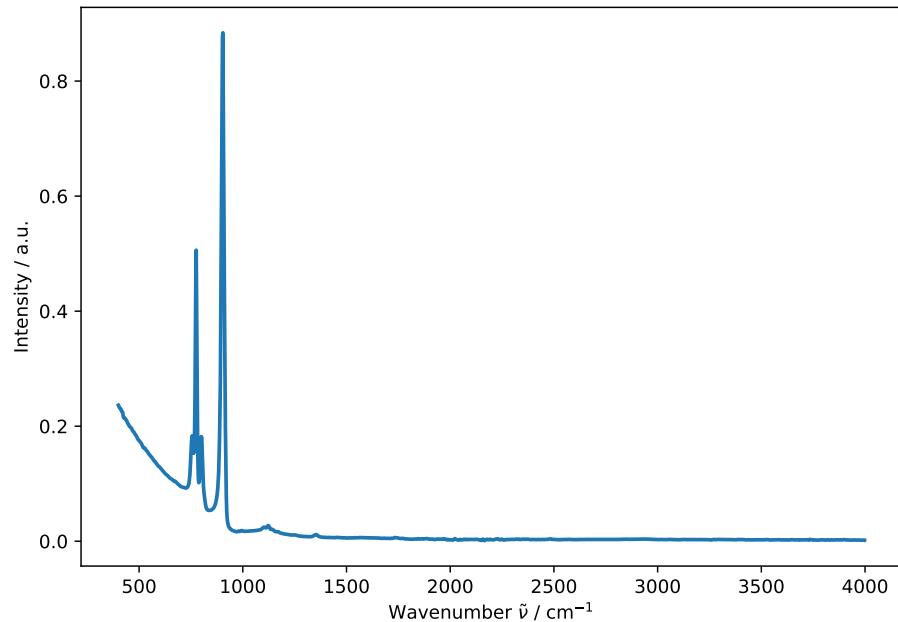


Fig. 9: Measured IR spectrum of tetrachloroethylene.

Tab. 21: Listed are the measured wavenumbers and intensities of the IR signals of C_2Cl_4 .

| signal | wavenumber $\tilde{\nu}$ / cm $^{-1}$ | intensity / a.u. |
|--------|---------------------------------------|------------------|
| 1 | 755.02 | 0.18 |
| 2 | 775.42 | 0.51 |
| 3 | 799.91 | 0.18 |
| 4 | 903.98 | 0.88 |
| 5 | 1122.32 | 0.03 |
| 6 | 1354.95 | 0.01 |

Tab. 22: Listed are the simulated wavenumbers and intensities of the vibrational modes of C_2Cl_4 .

| Mode | Wavenumber $\tilde{\nu}$ / cm^{-1} | Intensity / km mol^{-1} |
|------|---|----------------------------------|
| 1 | 97.18 | 0.00 |
| 2 | 174.89 | 0.96 |
| 3 | 234.77 | 0.00 |
| 4 | 286.90 | 0.51 |
| 5 | 310.42 | 0.03 |
| 6 | 342.99 | 0.00 |
| 7 | 447.02 | 0.00 |
| 8 | 514.19 | 0.00 |
| 9 | 774.46 | 82.16 |
| 10 | 895.52 | 202.05 |
| 11 | 978.50 | 0.00 |

3.8.2 Raman

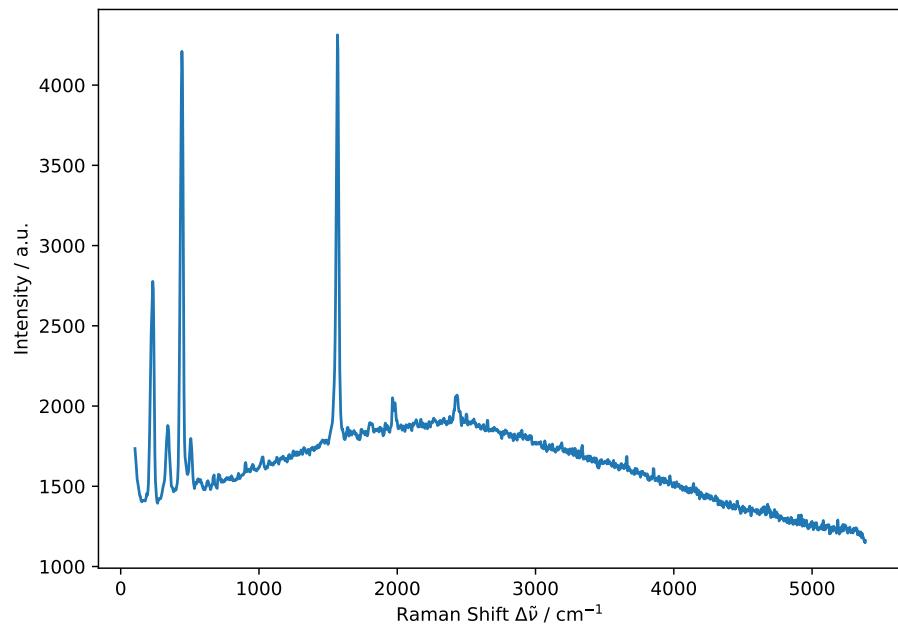


Fig. 10: Measured raman spectrum of tetrachloroethylene.

Tab. 23: Listed are the measured Raman shifts and intensities of the signals of C_2Cl_4 .

| signal | Raman Shift $\Delta\tilde{\nu}$ / cm^{-1} | intensity / a.u. |
|--------|--|------------------|
| 1 | 231.76 | 2776.67 |
| 2 | 339.67 | 1879.00 |
| 3 | 442.71 | 4210.33 |
| 4 | 1567.61 | 4313.00 |
| 5 | 2432.07 | 2068.33 |

Tab. 24: Listed are the simulated wavenumbers and Raman intensities of the vibrational modes of C_2Cl_4 .

| Mode | Wavenumber $\tilde{\nu}$ / cm^{-1} | Raman Intensity / $\text{\AA}^4 \text{ amu}^{-1}$ |
|------|---|---|
| 1 | 97.98 | 0.00 |
| 2 | 174.79 | 0.00 |
| 3 | 234.62 | 5.56 |
| 4 | 289.22 | 0.00 |
| 5 | 310.02 | 0.00 |
| 6 | 342.83 | 4.61 |
| 7 | 446.81 | 15.61 |
| 8 | 517.38 | 3.22 |
| 9 | 774.24 | 0.00 |
| 10 | 895.62 | 0.00 |
| 11 | 978.54 | 0.44 |
| 12 | 1623.90 | 48.63 |

4 Discussion

5 Conclusion

6 References

- [1] H. Dilger, *2025-pc2-script-en*, 2025.