IR + Raman - IR- and Raman-Spectroscopy

Protocol for the PC 2 lab course by

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Abstract:

Contents

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 analysized with the `WPenlighten` software. The IR spectra of dichloromethane, dibromomethane, chloroform and tetrachloroethylene were measured using an ATR spectrometer and analysized with the `Opus` software.

3 Results and Analysis

3.1 Methane

3.1.1 IR

3.1.2 Raman

3.2 Chloromethane

3.2.1 IR

3.2.2 Raman

3.3 Dichloromethane

3.3.1 IR

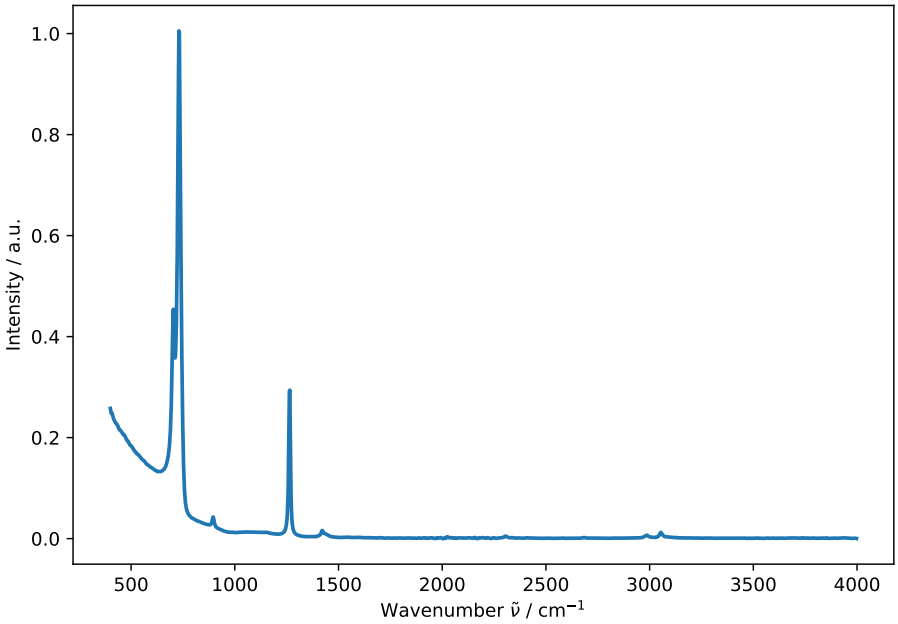

Figure 1: Measured IR spectrum of dichloromethane.

Table 1: 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

3.3.2 Raman

3.4 Dibromomethane

3.4.1 IR

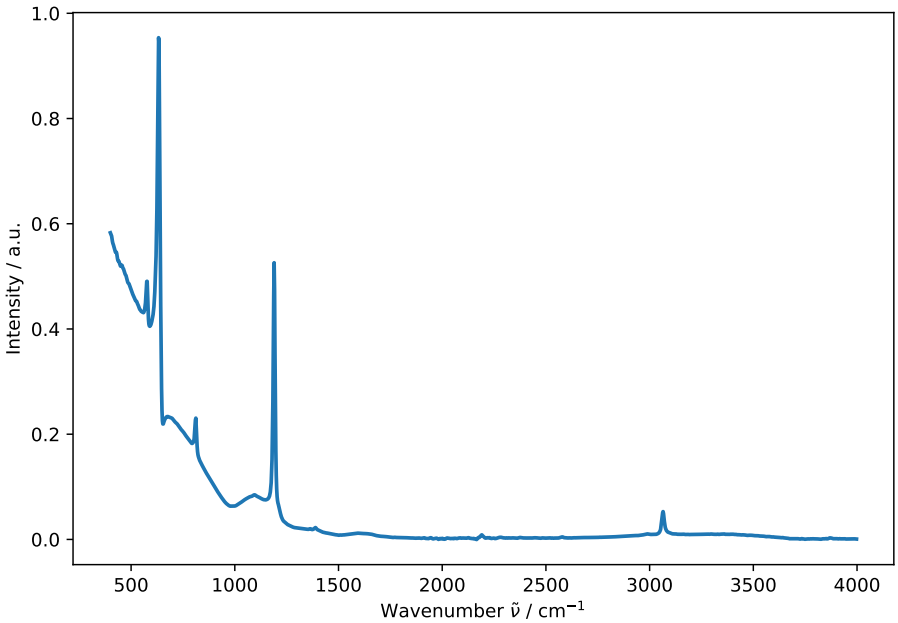

Figure 2: Measured IR spectrum of dibromomethane.

Table 2: 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

3.4.2 Raman

3.5 Chloroform

3.5.1 IR

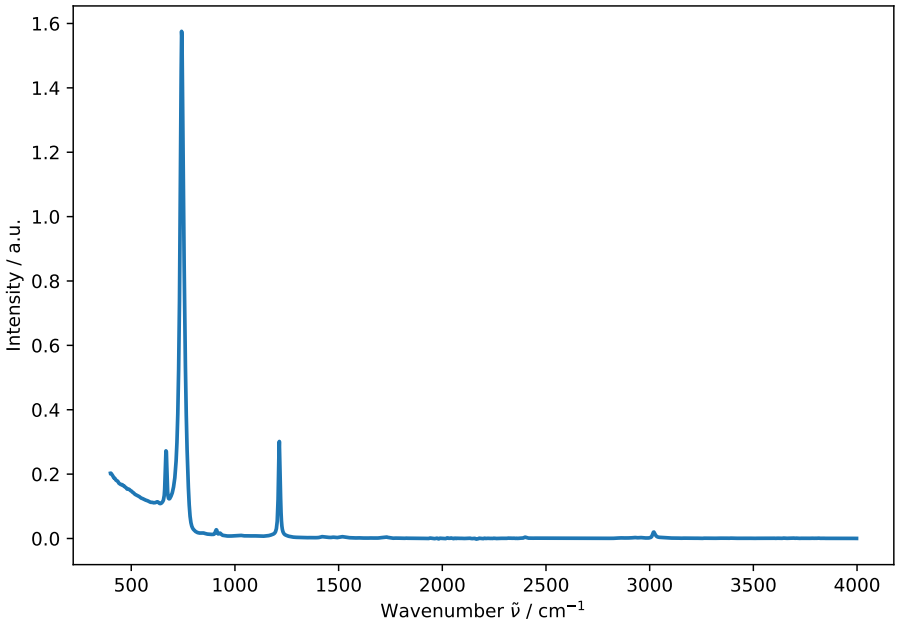

Figure 3: Measured IR spectrum of chloroform.

Table 3: Listed are the measured wavenumbers and intensities of the IR signals of $CHCl_3$.

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

3.5.2 Raman

3.6 Deuterated Chloroform

3.6.1 IR

3.6.2 Raman

3.7 Tetrachloromethane

3.7.1 IR

3.7.2 Raman

3.8 Tetrachloroethylene

3.8.1 IR

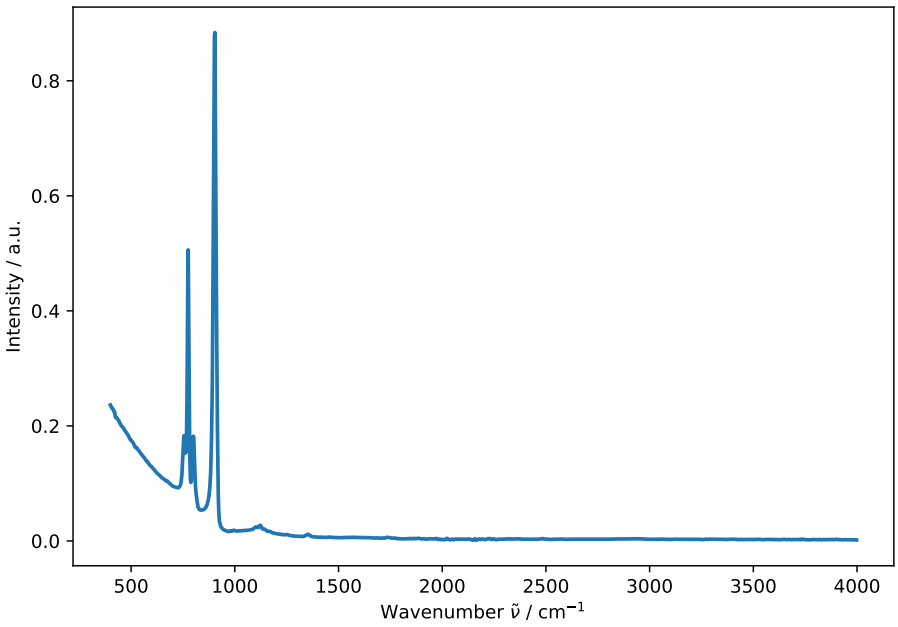

Figure 4: Measured IR spectrum of tetrachloroethylene.

Table 4: 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

3.8.2 Raman

4 Discussion

5 Conclusion

6 References

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