

IR + Raman - IR- and Raman-Spectroscopy

Protocol for the PC 2 lab course by
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date of experiment: 21.01.2026

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submission date: January 22, 2026

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

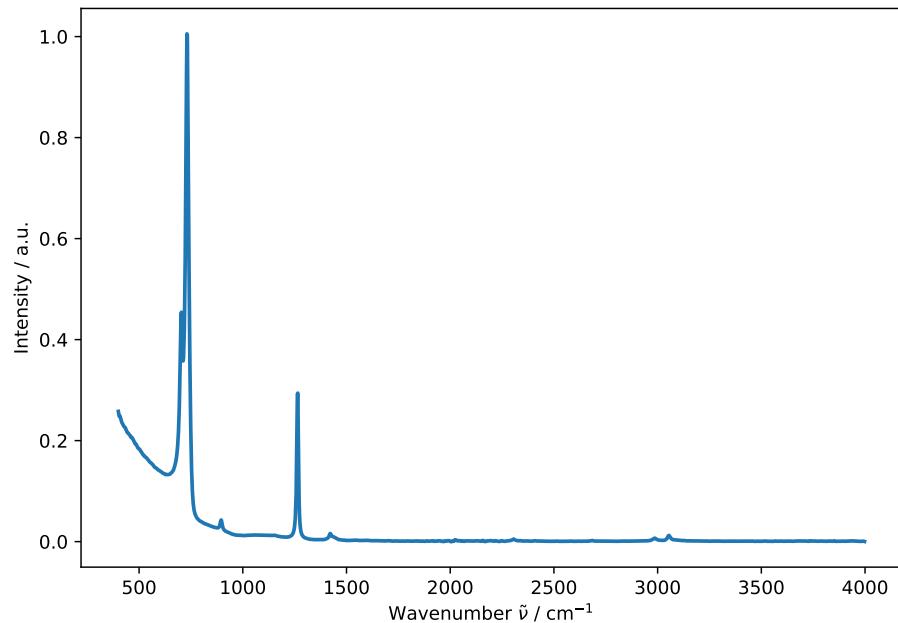


Fig. 1: Measured IR spectrum of dichloromethane.

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

3.3.2 Raman

3.4 Dibromomethane

3.4.1 IR

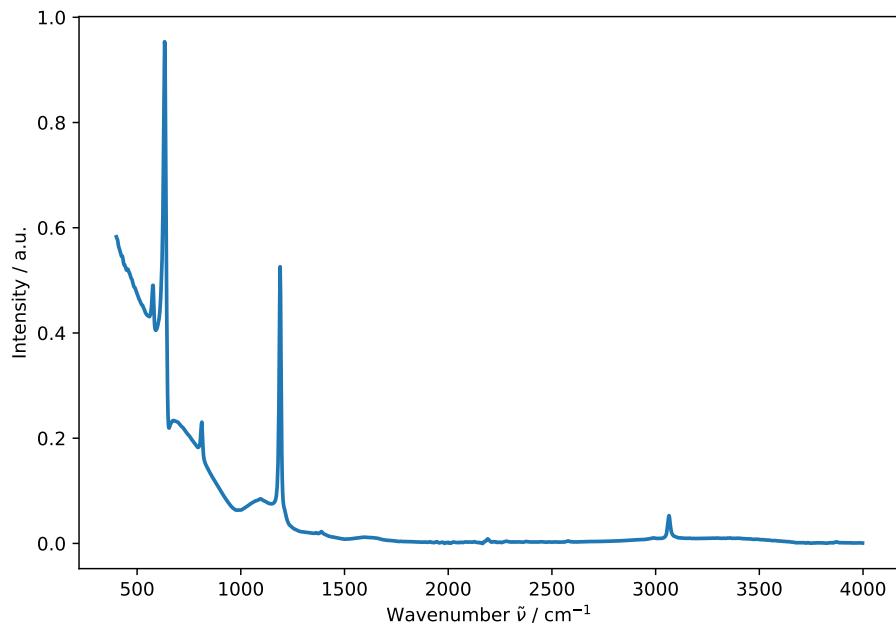


Fig. 2: Measured IR spectrum of dibromomethane.

Tab. 4: 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

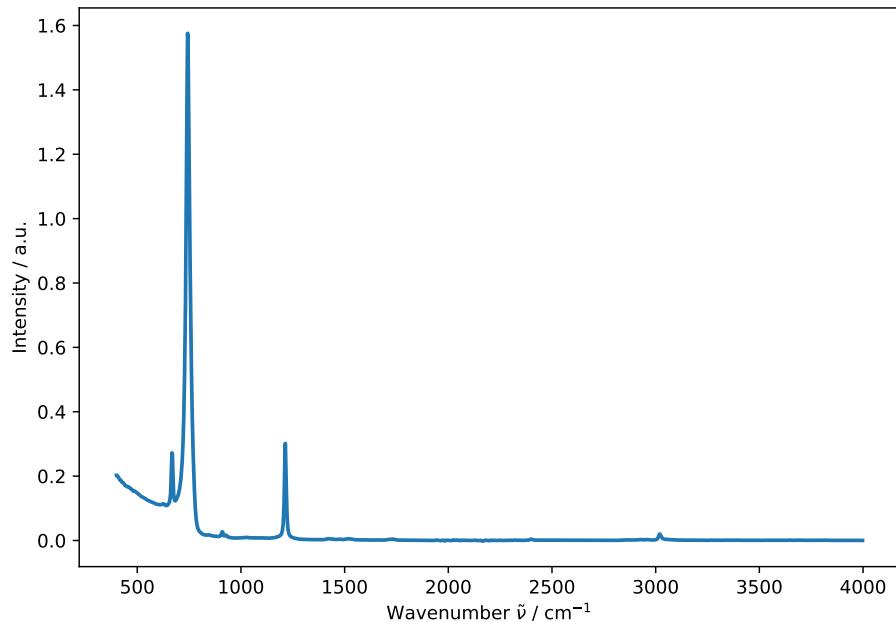


Fig. 3: Measured IR spectrum of chloroform.

Tab. 5: 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

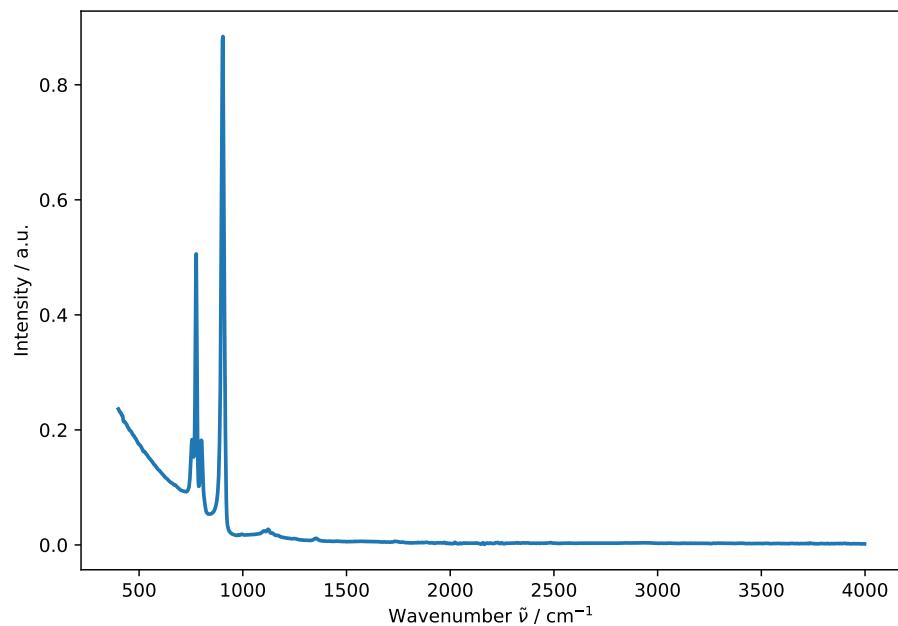


Fig. 4: Measured IR spectrum of tetrachloroethylene.

Tab. 6: Listed are the measured wavenumbers and intensities of the IR signals of C₂Cl₄.

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.