

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	2
3	Results and Analysis	2
3.1	Methane	2
3.1.1	IR	2
3.1.2	Raman	3
3.2	Chloromethane	4
3.2.1	IR	4
3.2.2	Raman	4
3.3	Dichloromethane	4
3.3.1	IR	4
3.3.2	Raman	5
3.4	Dibromomethane	6
3.4.1	IR	6
3.4.2	Raman	8
3.5	Chloroform	9
3.5.1	IR	9
3.5.2	Raman	11
3.6	Deuterated Chloroform	12
3.6.1	IR	12
3.6.2	Raman	13
3.7	Tetrachloromethane	14
3.7.1	IR	14
3.7.2	Raman	15
3.8	Tetrachloroethylene	16
3.8.1	IR	16
3.8.2	Raman	17
4	Discussion	18
5	Conclusion	18
6	References	18

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 CH₄ with the corresponding type of the vibrational mode.

signal	wavenumber $\tilde{\nu}$ / cm ⁻¹	intensity / KM·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

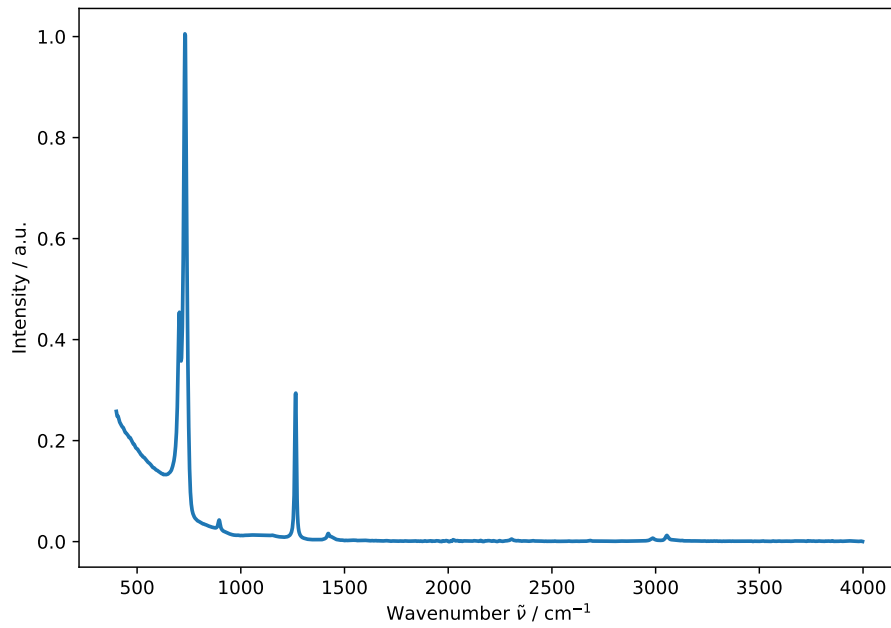


Fig. 1: Measured IR spectrum of dichloromethane.

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

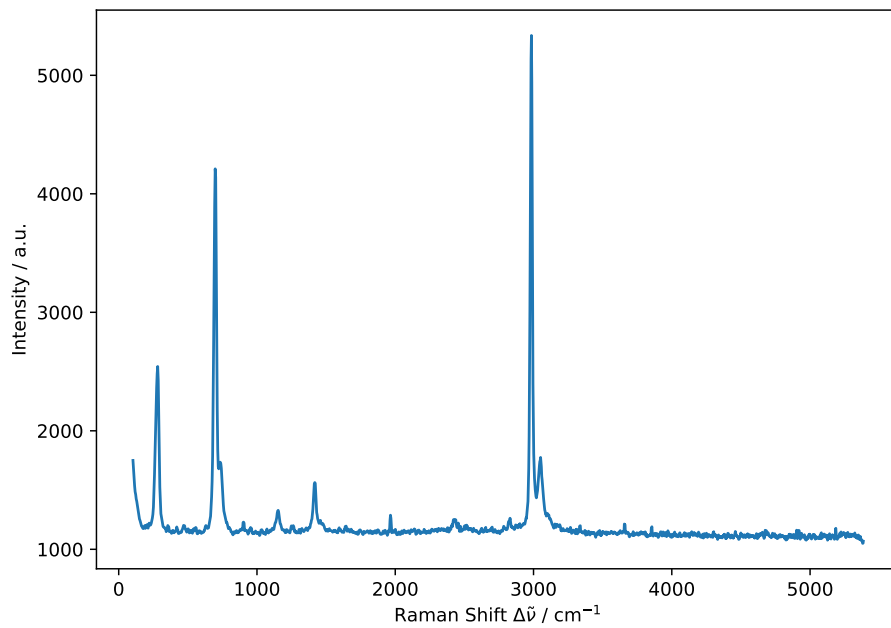


Fig. 2: Measured raman spectrum of dichloromethane.

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

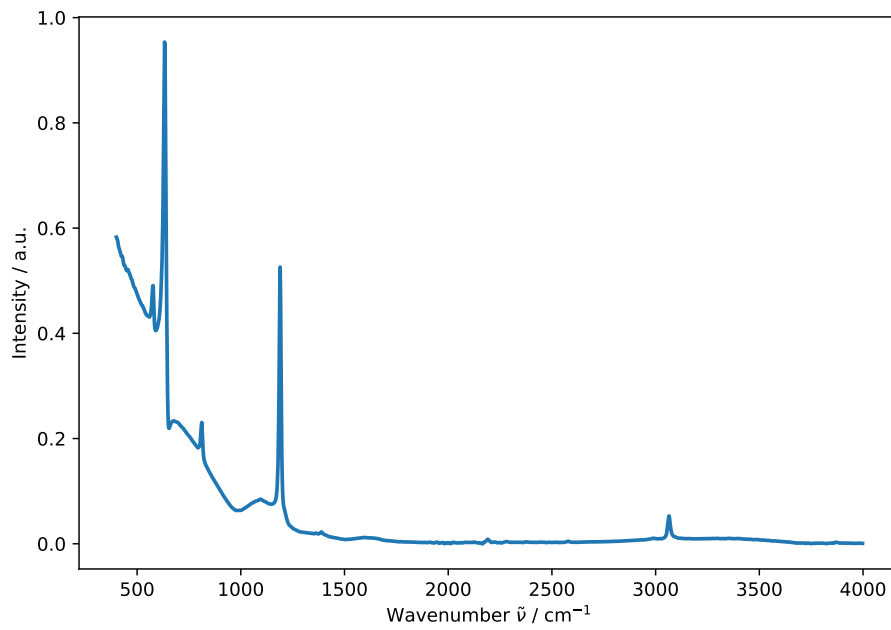


Fig. 3: Measured IR spectrum of dibromomethane.

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

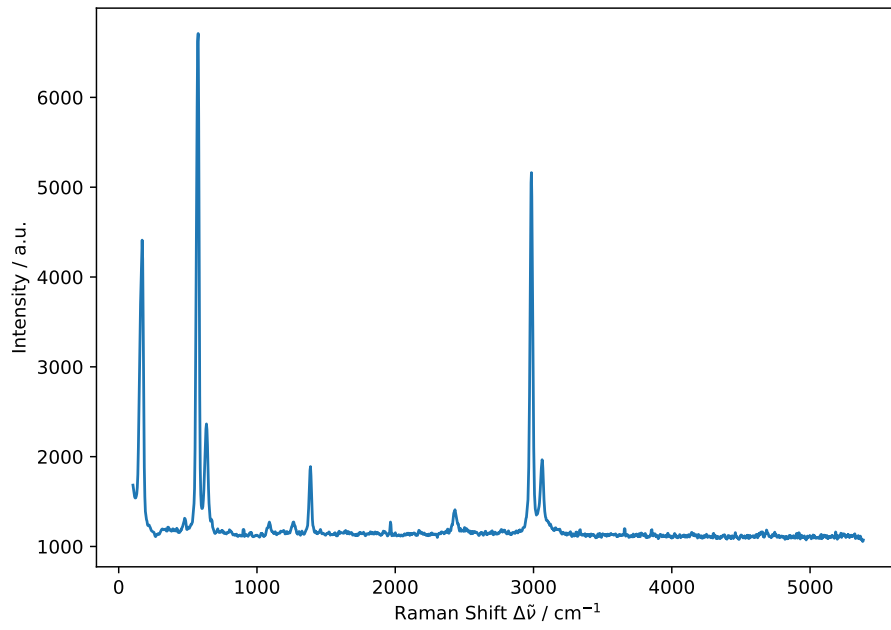


Fig. 4: Measured raman spectrum of dibromomethane.

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

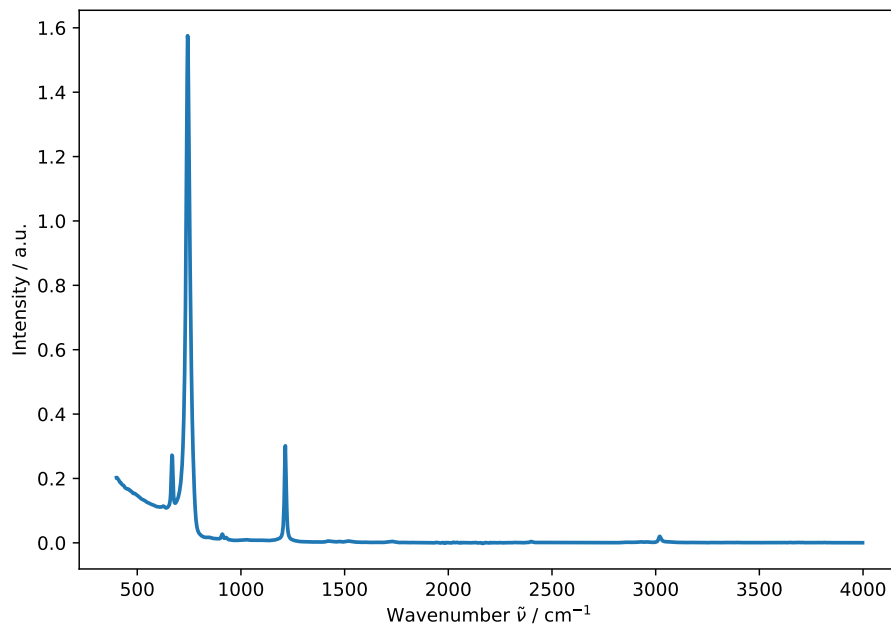


Fig. 5: Measured IR spectrum of chloroform.

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

Tab. 12: Listed are the simulated wavenumbers and intensities of the vibrational modes of CHCl_3 .

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

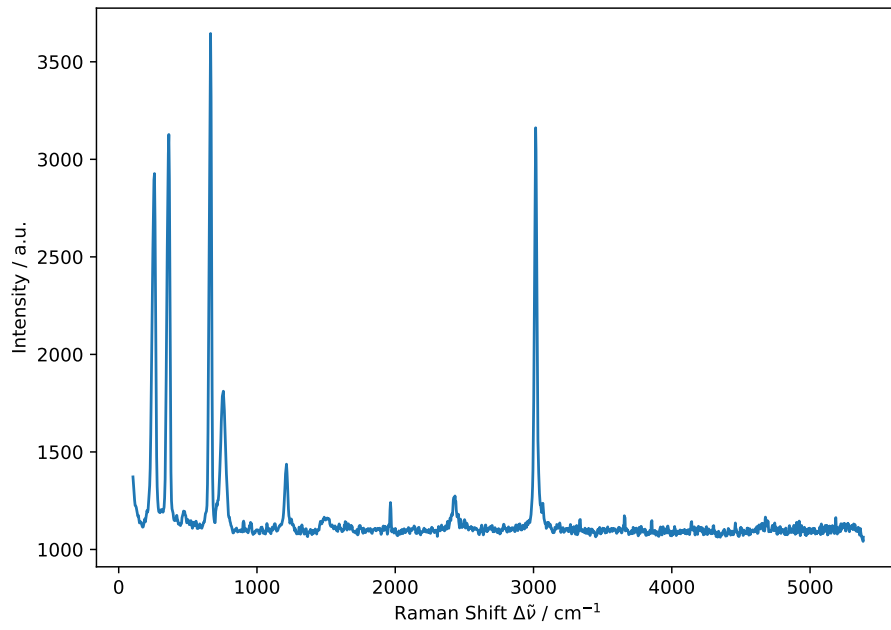


Fig. 6: Measured raman spectrum of chloroform.

Tab. 13: Listed are the measured Raman shifts and intensities of the signals of CHCl_3 .

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

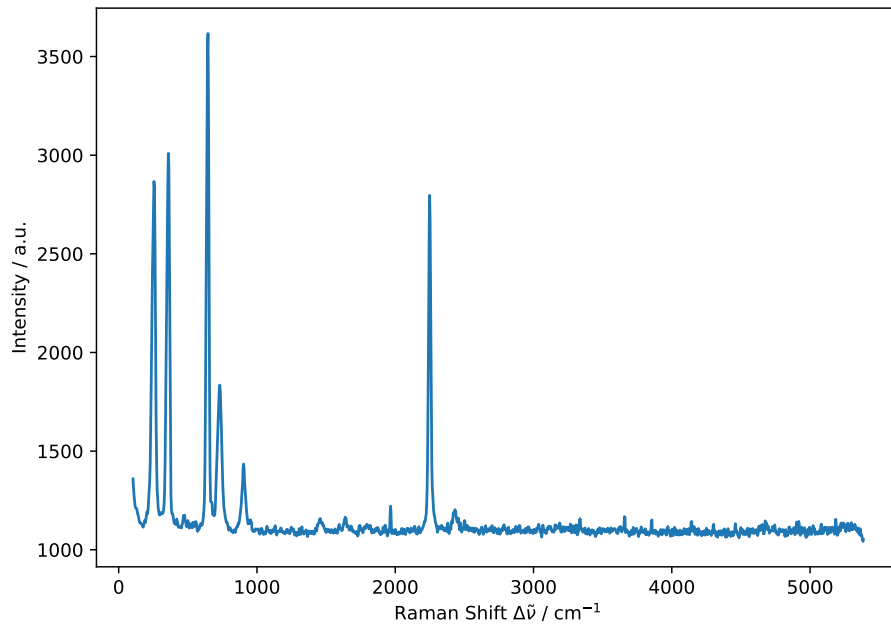


Fig. 7: Measured raman spectrum of deuterated chloroform.

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

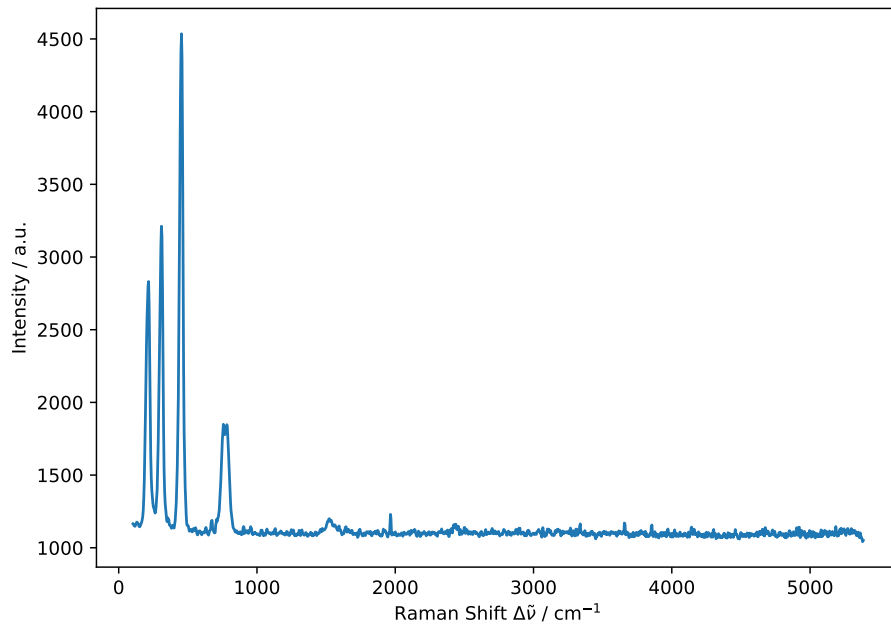


Fig. 8: Measured raman spectrum of tetrachloromethane.

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

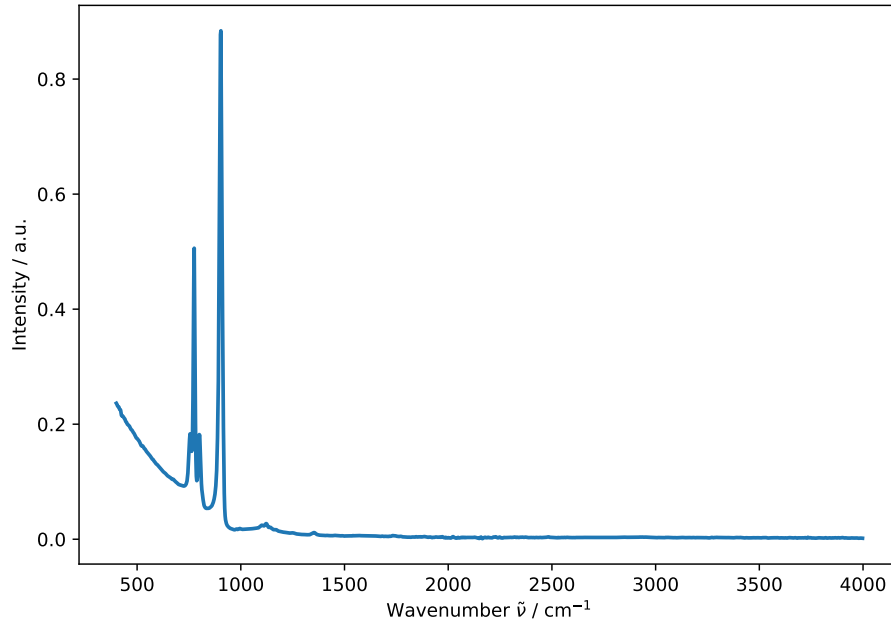


Fig. 9: Measured IR spectrum of tetrachloroethylene.

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

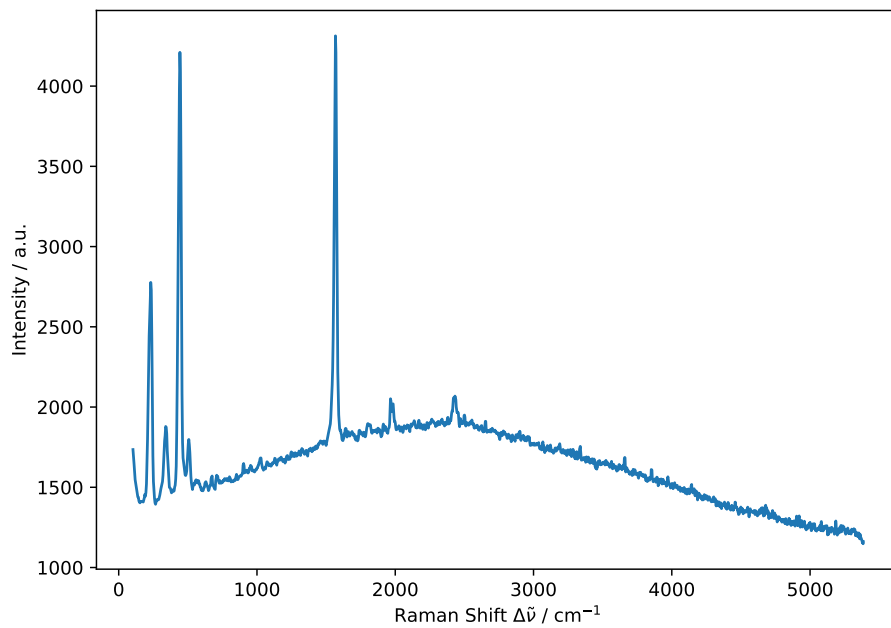


Fig. 10: Measured raman spectrum of tetrachloroethylene.

Tab. 23: Listed are the measured Raman shifts and intensities of the signals of C₂Cl₄.

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 C₂Cl₄.

Mode	Wavenumber $\tilde{\nu}$ / cm ⁻¹	Raman Intensity / Å ⁴ 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**.