

# IR + Raman - IR- and Raman-Spectroscopy

Protocol for the PC 2 lab course by  
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**Abstract:**

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# 1 Theory

## 1.1 IR-Spectroscopy

When a dipolar molecule is exposed to an electromagnetic field the partially positive charged atom is pushed along the direction of the magnetic field lines. So if a molecule is exposed to an oscillating field, that oscillates at the natural vibration frequency of said molecule, the molecule will be in an excited vibrational state.

## 1.2 Raman-Spectroscopy

## 1.3 DFT-Calculations

[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

The simulated vibrational modes of methane are summarized in Table 1 with the corresponding wavenumber, intensity and vibration type of each mode.

Tab. 1: Listed are the simulated wavenumbers and intensities of the IR signals of  $\text{CH}_4$  with the corresponding type of the vibrational mode.

Signal	Wavenumber $\tilde{\nu}$ / $\text{cm}^{-1}$	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

As can be seen in Table 1, only the asymmetric bending and stretching modes are IR-active, while the symmetric bending and stretching modes are IR-inactive. Furthermore, the asymmetric stretching mode shows the highest wavenumber among the IR-active modes, meaning it requires the most energy to be excited.

### 3.1.2 Raman

The simulated Raman-active vibrational modes of methane are summarized in ?? with the corresponding wavenumber, Raman intensity and vibration type of each mode.

Tab. 2: Listed are the simulated wavenumbers and intensities of the Raman signals of CH<sub>4</sub> with the corresponding type of the vibrational mode.

Mode	Raman shift $\Delta\tilde{\nu}$ / cm <sup>-1</sup>	Raman intensity / Å <sup>4</sup> · amu <sup>-1</sup>	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

In contrast to the IR spectrum, both the symmetric bending and stretching modes are Raman-active. The symmetric stretching mode shows the highest Raman intensity among all vibrational modes, indicating that it is most prominent mode to be observed in a Raman spectrum.

## 3.2 Chloromethane

### 3.2.1 IR

### 3.2.2 Raman

Tab. 3: Listed are the simulated Raman shifts and intensities of the vibrational modes of CH<sub>3</sub>Cl.

Mode	Raman Shift $\Delta\tilde{\nu}$ / cm <sup>-1</sup>	Raman intensity / Å <sup>4</sup> amu <sup>-1</sup>	vibration type
1	725.96	12.69	C–Cl stretch
2	1008.86	6.56	rocking
3	1010.02	6.53	rocking
4	1361.35	3.48	-
5	1455.81	16.49	-
6	1456.34	16.50	-
7	3056.94	134.62	sym. stretching
8	3169.78	66.78	asym. stretching
9	3170.01	66.72	asym. stretching

## 3.3 Dichloromethane

### 3.3.1 IR

The measured IR spectrum of dichloromethane is shown in Figure 1, plotting the intensity of the absorption against the wavenumber  $\tilde{\nu}$ .

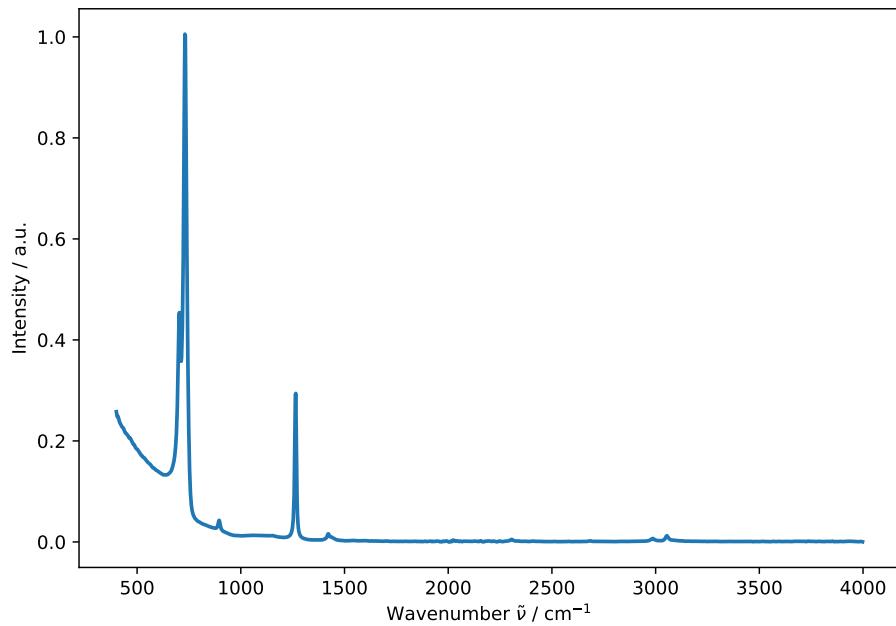


Fig. 1: Measured IR spectrum of dichloromethane.

By visual inspection of the IR spectrum in Figure 1, five absorption signals can be identified, which are listed with their corresponding wavenumbers and intensities in Table 4.

Tab. 4: Listed are the measured wavenumbers and intensities of the IR signals of  $\text{CH}_2\text{Cl}_2$  with the corresponding type of the vibrational mode. $\text{CH}_2\text{Cl}_2$ .

Signal	Wavenumber $\tilde{\nu}$ / $\text{cm}^{-1}$	Intensity / a.u.	Vibration type
1	704.00	0.45	sym. stretching
2	730.53	1.01	asym. stretching
3	895.82	0.04	rocking
4	1265.17	0.29	wagging
5	1422.29	0.02	scissoring

The simulated vibrational modes of dichloromethane are summarized in Table 5 with the corresponding wavenumber, intensity and vibration type of each mode.

Tab. 5: Listed are the simulated wavenumbers and intensities of the IR signals of  $\text{CH}_2\text{Cl}_2$  with the corresponding type of the vibrational mode.

Mode	Wavenumber $\tilde{\nu}$ / $\text{cm}^{-1}$	Intensity / $\text{KM}\cdot\text{mol}^{-1}$	Vibration type
1	277.23	0.64	-
2	703.86	14.19	sym. stretching
3	733.80	137.83	asym. stretching
4	889.17	1.20	rocking
5	1153.54	0.00	-
6	1272.86	41.21	wagging
7	1441.46	0.01	scissoring
8	3107.43	9.81	sym. stretching
9	3194.30	0.64	asym. stretching

As can be seen in Table 5, the most intense IR-active modes are found at wavenumbers of  $733.80 \text{ cm}^{-1}$  and  $1272.86 \text{ cm}^{-1}$ , which correspond well to the measured signals at  $730.53 \text{ cm}^{-1}$  for the asymmetric stretching mode and  $1265.17 \text{ cm}^{-1}$  for the wagging mode in Figure 1. The C-H stretching modes at around  $3100 \text{ cm}^{-1}$  calculated by ORCA are barely visible in Figure 1.

### 3.3.2 Raman

The measured Raman spectrum of dichloromethane is shown in Figure 2, plotting the Raman intensity against the Raman shift  $\Delta\tilde{\nu}$ .

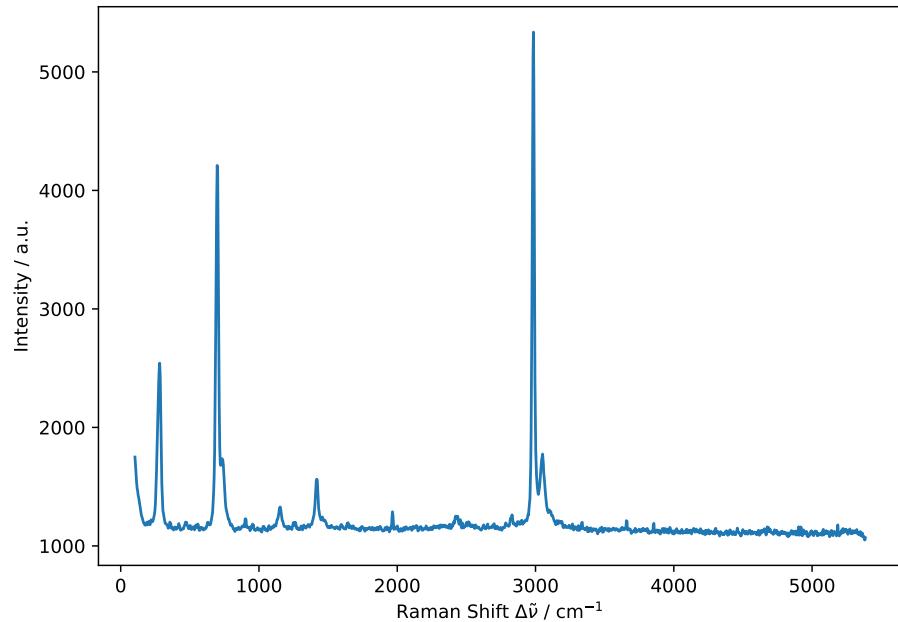


Fig. 2: Measured raman spectrum of dichloromethane.

By visual inspection of the Raman spectrum in Figure 2, five primary absorption signals can be identified, which are listed with their corresponding Raman shift, Raman intensity and vibration type of each mode.

Tab. 6: Listed are the measured Raman shifts and intensities of the signals of  $\text{CH}_2\text{Cl}_2$ .

Signal	Raman shift $\Delta\tilde{\nu}$ / $\text{cm}^{-1}$	intensity / a.u.	Vibration type
1	281.99	2542.67	scissoring
2	697.77	4210.67	sym. stretching
3	1418.07	1563.33	scissoring
4	2984.85	5336.00	sym. stretching
5	3051.13	1775.33	asym. stretching

The simulated Raman-active vibrational modes of dichloromethane are summarized in Table 7 with the corresponding Raman shift, Raman intensity and vibration type of each mode.

Tab. 7: Listed are the simulated Raman shifts and intensities of the vibrational modes of  $\text{CH}_2\text{Cl}_2$ .

Mode	Raman Shift $\Delta\tilde{\nu}$ / $\text{cm}^{-1}$	Raman intensity / $\text{\AA}^4 \text{amu}^{-1}$	Vibration type
1	277.06	6.83	scissoring
2	703.48	12.27	sym. stretching
3	732.67	5.02	asym. stretching
4	888.90	3.13	-
5	1153.83	11.78	-
6	1272.67	3.01	-
7	1441.64	12.42	scissoring
8	3106.65	108.70	sym. stretching
9	3193.09	62.65	asym. stretching

As can be seen in Table 6, the most intense Raman-active modes are found at wavenumbers of  $281.99 \text{ cm}^{-1}$ ,  $697.77 \text{ cm}^{-1}$  and  $2984.85 \text{ cm}^{-1}$ , which correspond to the calculated signals at  $277.06 \text{ cm}^{-1}$  for the scissoring mode and  $703.48 \text{ cm}^{-1}$  for the symmetric stretching mode in Table 7. But similar to the IR spectrum, the wavenumbers of the C-H stretching modes in the measured Raman spectrum at  $2984.85 \text{ cm}^{-1}$  and  $3051.13 \text{ cm}^{-1}$  deviate by approximately  $130 \text{ cm}^{-1}$  from the calculated values of  $3106.65 \text{ cm}^{-1}$  and  $3193.09 \text{ cm}^{-1}$ .

### 3.4 Dibromomethane

#### 3.4.1 IR

The measured IR spectrum of dibromomethane is shown in Figure 3, plotting the intensity of the absorption against the wavenumber  $\tilde{\nu}$ .

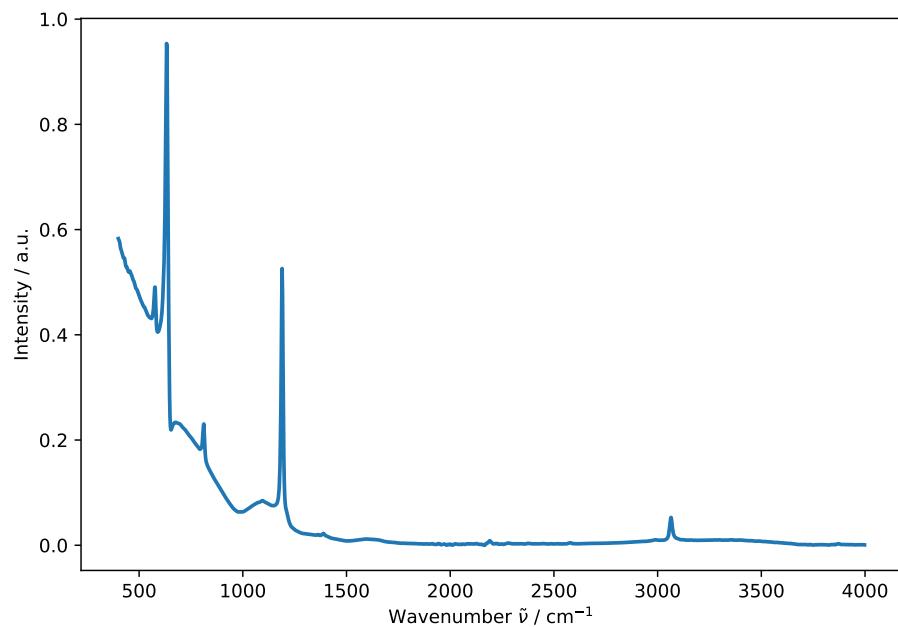


Fig. 3: Measured IR spectrum of dibromomethane.

Tab. 8: Listed are the measured wavenumbers and intensities of the IR signals of  $\text{CH}_2\text{Br}_2$ .

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. 9: Listed are the simulated wavenumbers and intensities of the vibrational modes of  $\text{CH}_2\text{Br}_2$ .

Mode	Wavenumber $\tilde{\nu}$ / $\text{cm}^{-1}$	Intensity / $\text{KM}\cdot\text{mol}^{-1}$
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

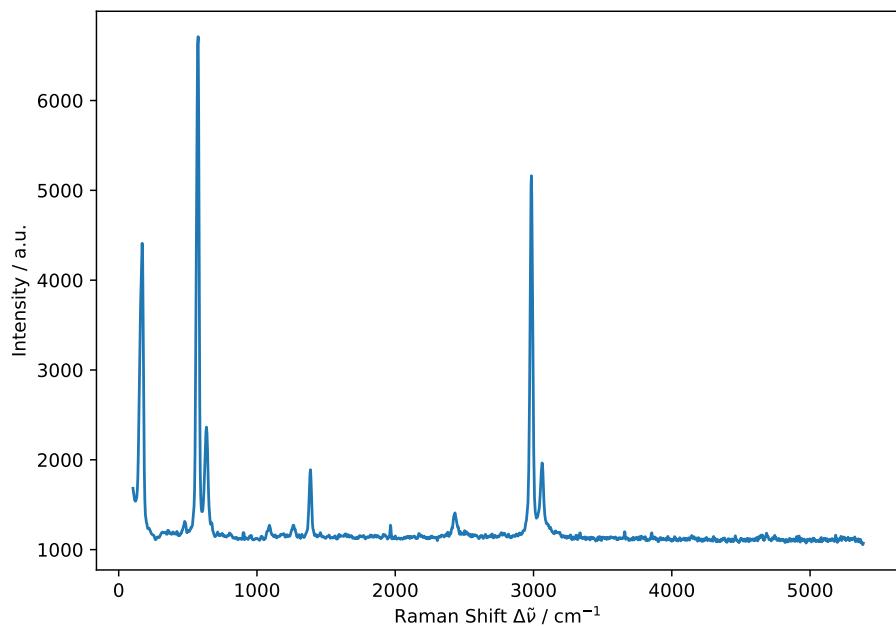


Fig. 4: Measured raman spectrum of dibromomethane.

Tab. 10: Listed are the measured Raman shifts and intensities of the signals of  $\text{CH}_2\text{Br}_2$ .

Signal	Raman shift $\Delta\tilde{\nu}$ / $\text{cm}^{-1}$	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. 11: Listed are the simulated wavenumbers and raman intensities of the vibrational modes of  $\text{CH}_2\text{Br}_2$ .

Mode	Wavenumber $\tilde{\nu}$ / $\text{cm}^{-1}$	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

The measured IR spectrum of chloroform is shown in Figure 5, plotting the intensity of the absorption against the wavenumber  $\tilde{\nu}$ .

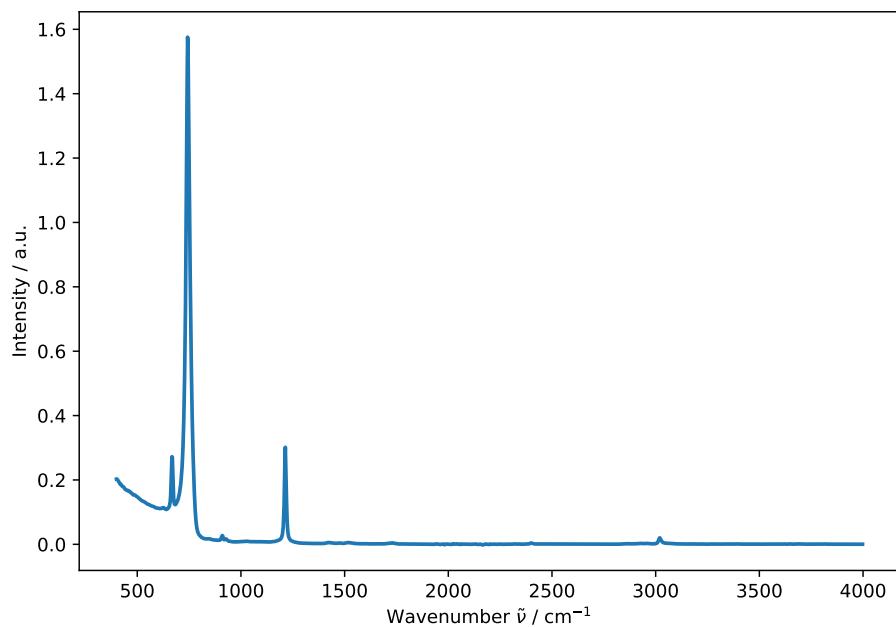


Fig. 5: Measured IR spectrum of chloroform.

Tab. 12: Listed are the measured wavenumbers and intensities of the IR signals of CHCl<sub>3</sub>.

Signal	Wavenumber $\tilde{\nu}$ / cm <sup>-1</sup>	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. 13: Listed are the simulated wavenumbers and intensities of the vibrational modes of CHCl<sub>3</sub>.

Mode	Wavenumber $\tilde{\nu}$ / cm <sup>-1</sup>	Intensity / KM·mol <sup>-1</sup>
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

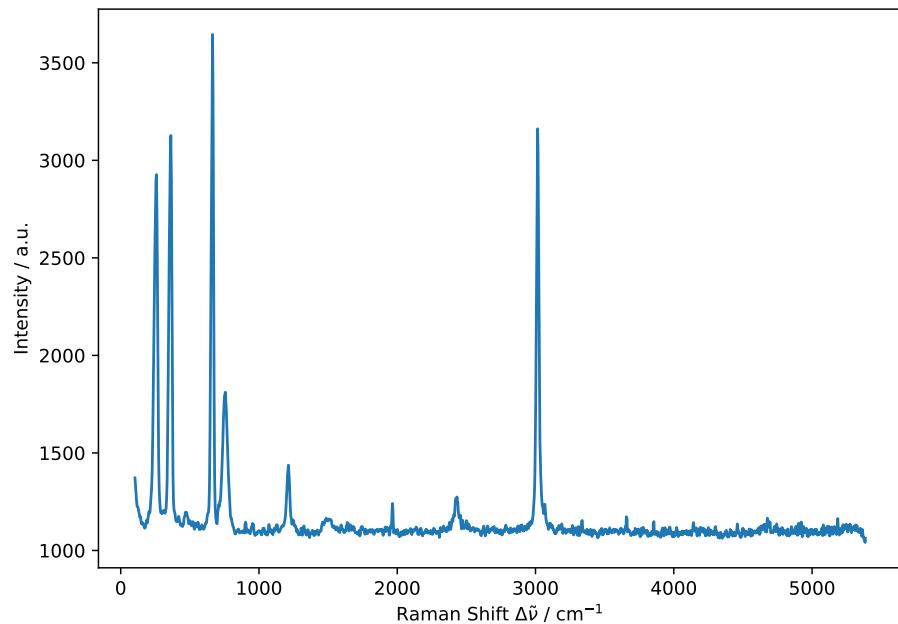


Fig. 6: Measured raman spectrum of chloroform.

Tab. 14: Listed are the measured Raman shifts and intensities of the signals of CHCl<sub>3</sub>.

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. 15: Listed are the simulated wavenumbers and raman intensities of the vibrational modes of  $\text{CHCl}_3$ .

Mode	Wavenumber $\tilde{\nu}$ / $\text{cm}^{-1}$	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. 16: Listed are the simulated wavenumbers and intensities of the vibrational modes of  $\text{CDCl}_3$ .

Mode	Wavenumber $\tilde{\nu}$ / $\text{cm}^{-1}$	Intensity / $\text{KM}\cdot\text{mol}^{-1}$
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

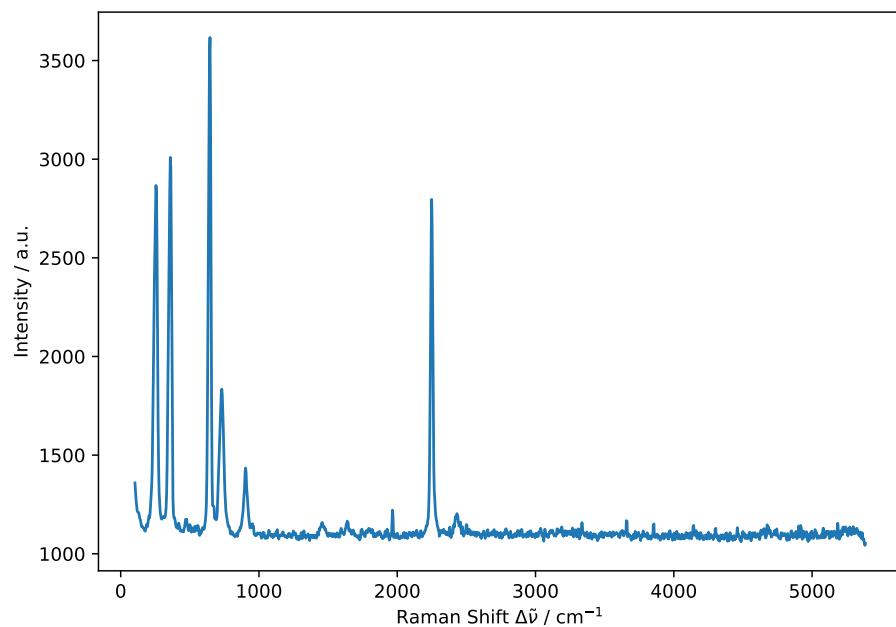


Fig. 7: Measured raman spectrum of deuterated chloroform.

Tab. 17: Listed are the measured Raman shifts and intensities of the signals of  $\text{CDCl}_3$ .

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. 18: Listed are the simulated wavenumbers and raman intensities of the vibrational modes of  $\text{CDCl}_3$ .

Mode	Wavenumber $\tilde{\nu}$ / $\text{cm}^{-1}$	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. 19: Listed are the simulated wavenumbers and intensities of the vibrational modes of  $\text{CCl}_4$ .

Mode	Wavenumber $\tilde{\nu}$ / $\text{cm}^{-1}$	Intensity / $\text{KM} \cdot \text{mol}^{-1}$
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

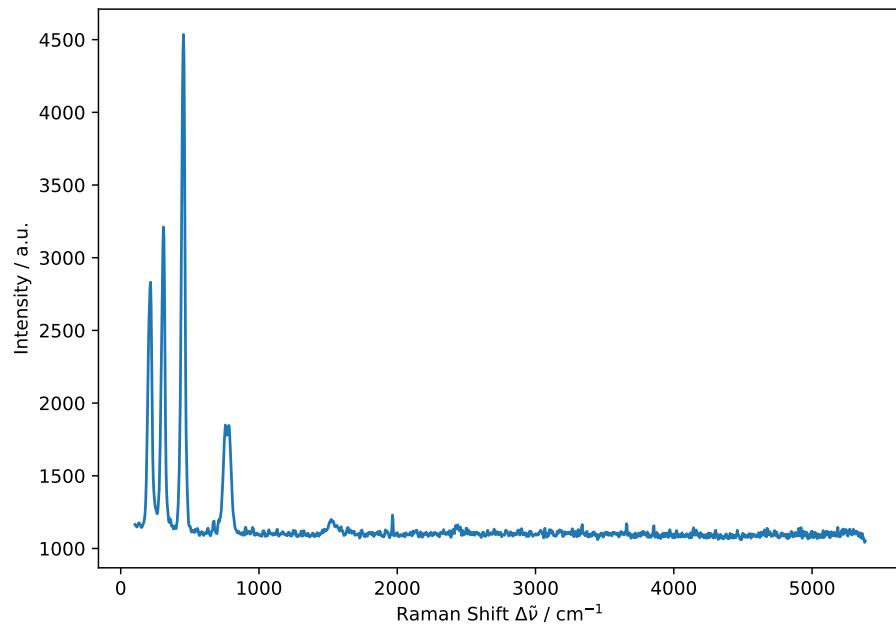


Fig. 8: Measured raman spectrum of tetrachloromethane.

Tab. 20: Listed are the measured Raman shifts and intensities of the signals of  $\text{CCl}_4$ .

Signal	Raman shift $\Delta\tilde{\nu}$ / $\text{cm}^{-1}$	Intensity / a.u.
1	216.25	2831.33
2	308.95	3211.67
3	454.10	4535.33
4	756.86	1849.33

Tab. 21: Listed are the simulated wavenumbers and Raman intensities of the vibrational modes of  $\text{CCl}_4$ .

Mode	Wavenumber $\tilde{\nu}$ / $\text{cm}^{-1}$	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

The measured IR spectrum of tetrachloroethylene is shown in Figure 9, plotting the intensity of the absorption against the wavenumber  $\tilde{\nu}$ .

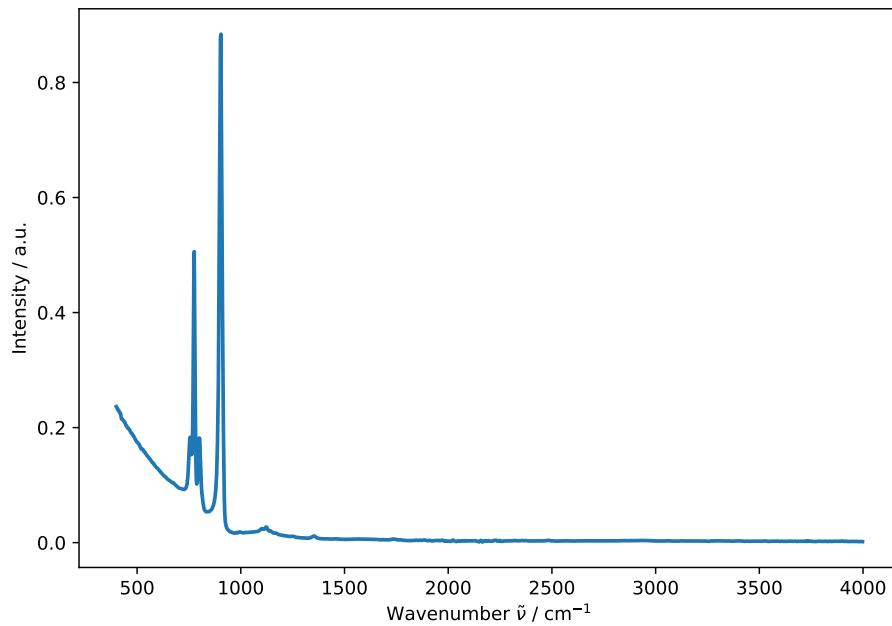


Fig. 9: Measured IR spectrum of tetrachloroethylene.

By visual inspection of the IR spectrum in Figure 9, six absorption signals can be identified, which are listed with their corresponding wavenumbers and intensities in Table 22.

Tab. 22: Listed are the measured wavenumbers and intensities of the IR signals of  $\text{C}_2\text{Cl}_4$  with the corresponding type of the vibrational mode.

Signal	Wavenumber $\tilde{\nu}$ / cm <sup>-1</sup>	Intensity / a.u.	Vibration type
1	755.02	0.18	
2	775.42	0.51	asym. C-Cl stretching
3	799.91	0.18	
4	903.98	0.88	asym. C-Cl stretching
5	1122.32	0.03	
6	1354.95	0.01	

The simulated vibrational modes of tetrachloroethylene are summarized in Table 23 with the corresponding wavenumber, intensity and vibration type of each mode.

Tab. 23: Listed are the simulated wavenumbers and intensities of the vibrational modes of  $\text{C}_2\text{Cl}_4$ .

Mode	Wavenumber $\tilde{\nu}$ / $\text{cm}^{-1}$	Intensity / $\text{KM}\cdot\text{mol}^{-1}$	Vibration type
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	asym. C-Cl stretch
10	895.52	202.05	asym. C-Cl stretch
11	978.50	0.00	

As can be seen in Table 23, the most intense IR-active modes are found at wavenumbers of  $774.46 \text{ cm}^{-1}$  and  $895.52 \text{ cm}^{-1}$ , which correspond well to the measured signals at  $755.02 \text{ cm}^{-1}$  and  $903.98 \text{ cm}^{-1}$  in Figure 9.

In comparison to the simulated IR spectrum of chloroform with the wavenumbers and vibrational modes in Table 12, tetrachloroethylene shows additional IR-active modes in the low wavenumber region below  $500 \text{ cm}^{-1}$ , which can be attributed to the increased number of atoms in the molecule leading to more vibrational modes.

### 3.8.2 Raman

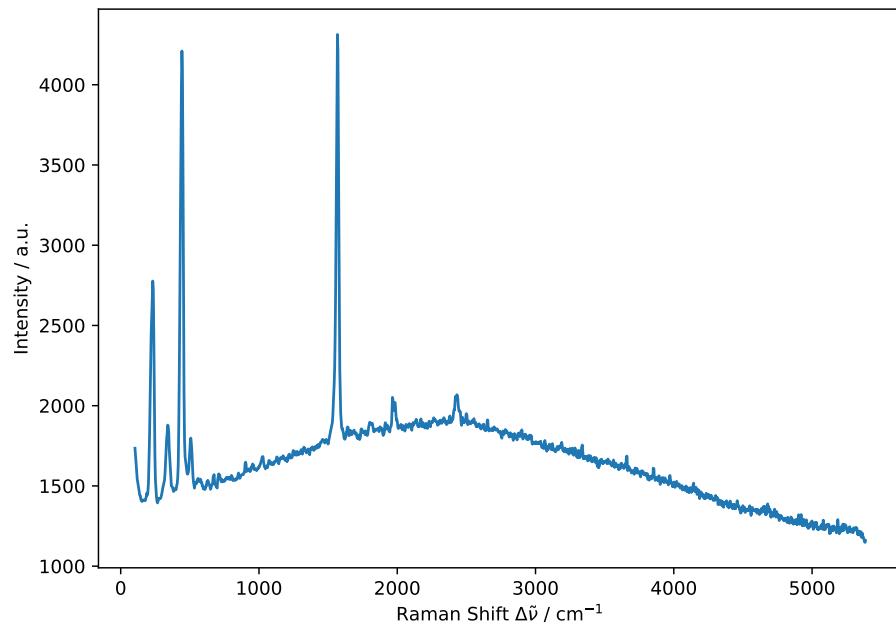


Fig. 10: Measured raman spectrum of tetrachloroethylene.

Tab. 24: 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.	Vibration type
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. 25: Listed are the simulated wavenumbers and Raman intensities of the vibrational modes of  $\text{C}_2\text{Cl}_4$ .

Mode	Wavenumber $\tilde{\nu}$ / $\text{cm}^{-1}$	Raman intensity / $\text{\AA}^4 \text{amu}^{-1}$	Vibration type
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	asym. C-Cl stretch
10	895.62	0.00	asym. C-Cl stretch
11	978.54	0.44	
12	1623.90	48.63	C=C stretching

In comparison to the simulated IR-active modes in Table 23, Table 25 shows that the most intense Raman-active mode is found at a wavenumber of  $1623.90 \text{ cm}^{-1}$ , which can be assigned to the  $\text{C} = \text{C}$  stretching mode of tetrachloroethylene, which is not present in the simulated IR spectrum. The cause for this lies in the rule of mutual exclusion, which applies to molecules with a center of symmetry, such as the inversion center of tetrachloroethylene. According to this rule, vibrational modes that are Raman-active are IR-inactive and vice versa, explaining the absence of the  $1623.90 \text{ cm}^{-1}$  mode in the IR spectrum. By comparing the simulated Raman modes of  $\text{C}_2\text{Cl}_4$  from Table 25 with the simulated Raman modes of  $\text{CHCl}_3$  in Table 14, the structural differences between the two molecules can be explained. While both molecules show Raman-active modes in the low wavenumber region below  $500 \text{ cm}^{-1}$ , tetrachloroethylene exhibits an additional strong Raman-active mode at  $1623.90 \text{ cm}^{-1}$ , which can be attributed to the presence of the  $\text{C} = \text{C}$  double bond in  $\text{C}_2\text{Cl}_4$  that is absent in  $\text{CHCl}_3$ . Additionally, the C-H stretching mode at  $3168.77 \text{ cm}^{-1}$  present in chloroform is not observed in tetrachloroethylene due to the lack of hydrogen atoms in its structure.

## 4 Discussion

By plotting the calculated Raman shifts against the vibrational mode number for Methane and all Chloromethanes from Table 2, Table 3, Table 7, Table 15 and Table 21, the Raman trends of the investigated molecules can be visualized in Figure 11.

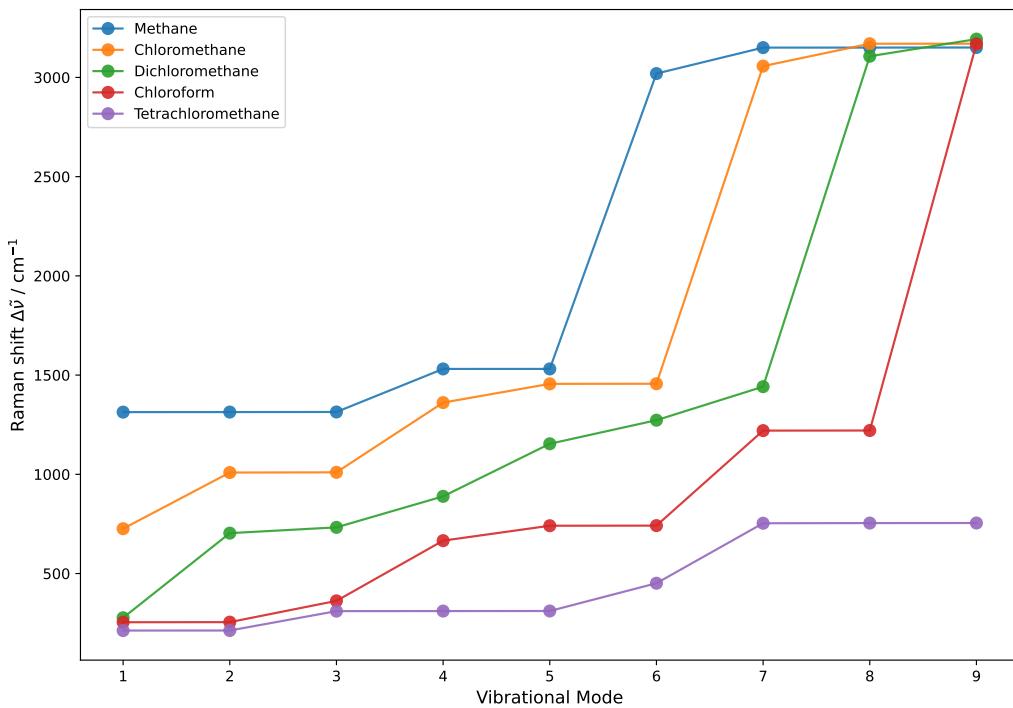


Fig. 11: Raman shifts plotted against the vibrational mode number for  $\text{CH}_4$ ,  $\text{CH}_3\text{Cl}$ ,  $\text{CH}_2\text{Cl}_2$ ,  $\text{CHCl}_3$  and  $\text{CCl}_4$ .

The first trend noticeable in Figure 11 is the decrease of the Raman shifts with increasing number of chlorine atoms in the molecule. This can be explained by the increasing reduced mass  $\mu$  of the molecules due to the substitution of hydrogen atoms (mass = 1 u) with chlorine atoms (mass = 35.5 u), leading to lower vibrational frequencies  $\tilde{\nu}$  according to Equation 1.

$$\tilde{\nu} = \nu \cdot c = \sqrt{\frac{k}{\mu}} \quad (1)$$

Following that argumentation, the number of vibrational modes at around  $3000 \text{ cm}^{-1}$ , which can be assigned to the C-H stretching vibrations, decreases with increasing number of chlorine atoms in the molecule until no C-H stretching modes are present in tetrachloromethane due to the absence of hydrogen atoms in its structure. In return, new vibrational modes appear in the low wavenumber region below  $1000 \text{ cm}^{-1}$ , which can be assigned to the C-Cl stretching vibrations. Another trend observable in Figure 11 is that methane and tetrachloromethane show more vibrational modes with nearly the same Raman shift compared to the other chloromethanes. This can be explained by the high symmetry of both molecules, which belong to the tetrahedral point group  $T_d$ . This trend is especially visible in the triply degenerate asymmetric stretching vibration of methane at  $3150 \text{ cm}^{-1}$  and tetrachloromethane at  $754 \text{ cm}^{-1}$ .

## **5 Conclusion**

## **6 References**

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