

# **Abgabe Blatt 5**

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# 1 Evaluation

## 1.1 Raman

For the following Raman spectra, the selection rule applies, that the polarizability of the molecule needs to change with the absorption. This means only those vibrational modes are Raman active and will thus be visible in the spectrum, which are linked to a change in the dipole of the molecule. [1]

### 1.1.1 Comparison of experimental and calculated spectra

The calculated and measured peak positions for the chloroform are listed in table (1)

Table 1: Theoretically calculated peak positions  $\tilde{\nu}_{\text{theo}}$  with their activity  $A$  and depolarisation  $\rho$  and experimentally measured peak positions  $\tilde{\nu}_{\text{exp}}$  with their intensity  $I$  for chloroform.

Mode	$\tilde{\nu}_{\text{theo}}$	$A$	$\rho$	$\tilde{\nu}_{\text{exp}}$	$I$
6	254.65	5.14	0.75	-	-
7	254.97	5.13	0.75	402.08	2913.67
8	361.89	8.68	0.24	492.15	3156.67
9	665.44	9.80	0.00	-	-
10	740.53	3.09	0.75	759.03	3644.33
11	740.76	3.08	0.75	839.09	1774
12	1219.78	6.03	0.75	-	-
13	1220.55	6.02	0.75	1266.11	1429
14	3168.76	77.21	0.24	3187.65	3136

It is clearly visible that the experimental data follow the Raman selection rules, as vibrational mode 9 is not observable. Additionally, deviations in the wavenumbers are seen between the simulated and experimental data. Furthermore, there are several simulated peaks that possess similar wavenumbers and are superimposed in the experimental data due to line broadening.

The recorded spectrum for chloroform is depicted in figure (1).

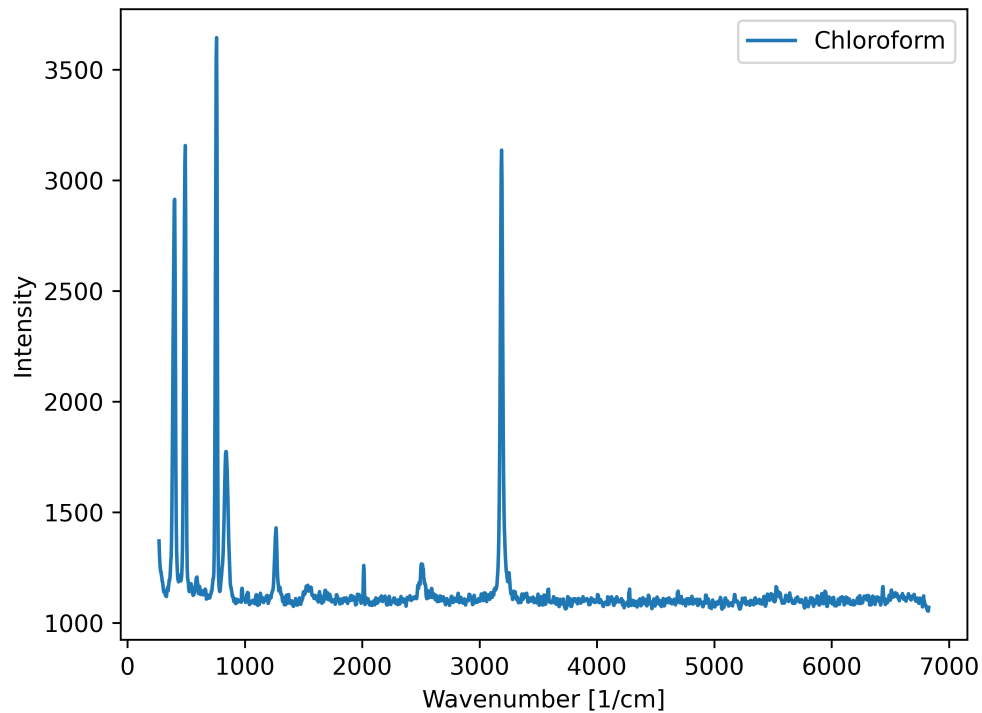


Figure 1: Raman spectrum of Chloroform.

In this plot, 8 peaks are visible, 4 of which at a wavenumber lower than  $1000\text{ cm}^{-1}$ , one at around  $1200\text{ cm}^{-1}$  and one at around  $3000\text{ cm}^{-1}$ . The one at  $2500\text{ cm}^{-1}$  must be caused by impurifications. The peak at  $2000\text{ cm}^{-1}$  is the Rayleigh peak which is present in all the following spectra.

$$\frac{\sqrt{\tilde{\mu}_{\text{H}}}}{\sqrt{\tilde{\mu}_{\text{D}}}} = \frac{0.923\text{ u}}{1.714\text{ u}} = 0.538 \quad (1.1)$$

Mit der Formel (1.1) kann das Verhältnis der der C-H zur C-D Schwinung berechnet werden, wofür sich in diesem Beispiel ein Verhältnis von 0.539.

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## 2 References

- [1] J. van Slageren H. Dilger. *Script for the PC II Lab Course*.