

# Beispiel: Strukturbestimmung

Erwartungsspektren:

Anzahl, Lage und Intensität der Banden;  
Depolarisationsgrad

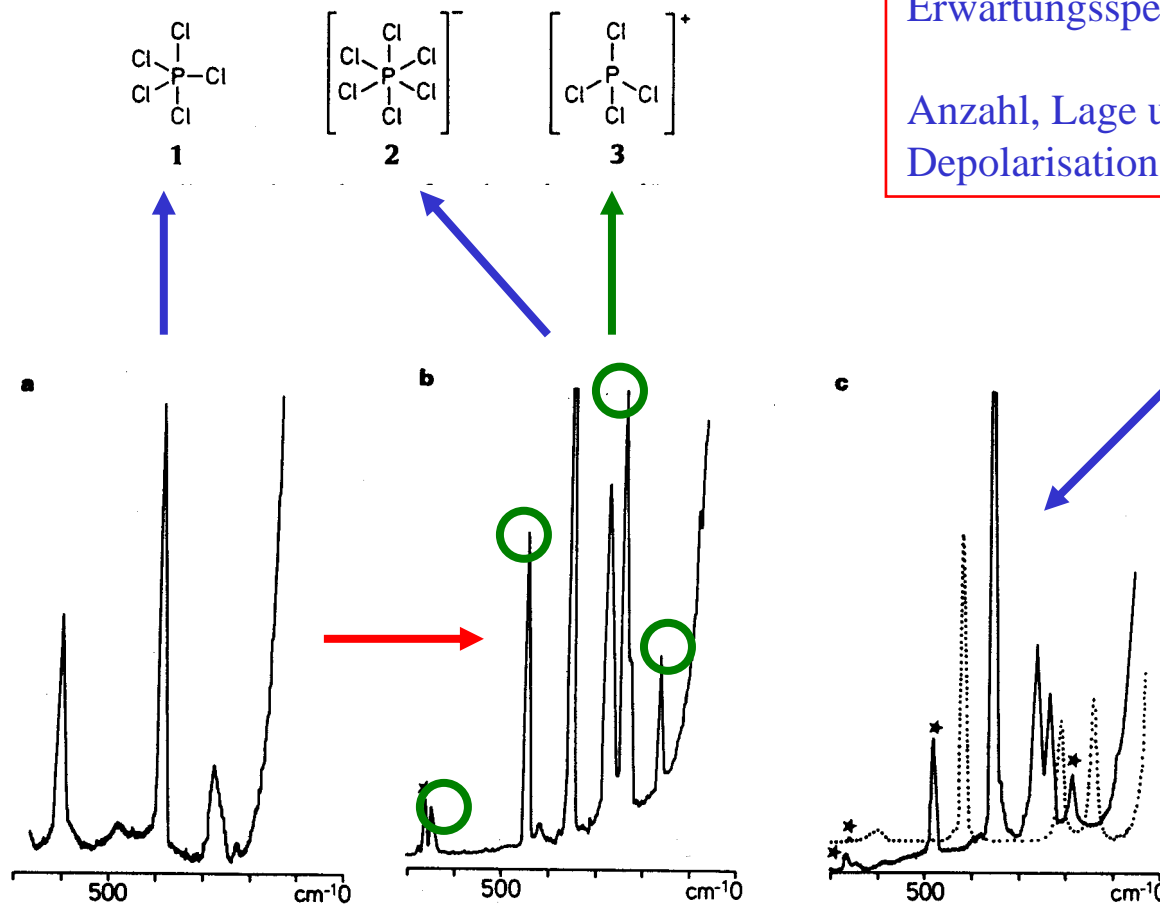


Abb. 14.10 Ramanspektren von  $\text{PCl}_5$  und Vergleichssubstanzen.

- a  $\text{PCl}_5$  in Lösung (Benzol),
- b  $\text{PCl}_5$  kristallin,
- c —  $\text{PCl}_6^-$  in Lösung ( $\text{PCl}_5$  in  $\text{CH}_3[\text{C}_2\text{H}_5]_3\text{NCl}$ ),  
 .....  $\text{SiCl}_4(\text{fl.})$ ,
- \* Fremdbanden

# Beispiel: Rotationsisomerie

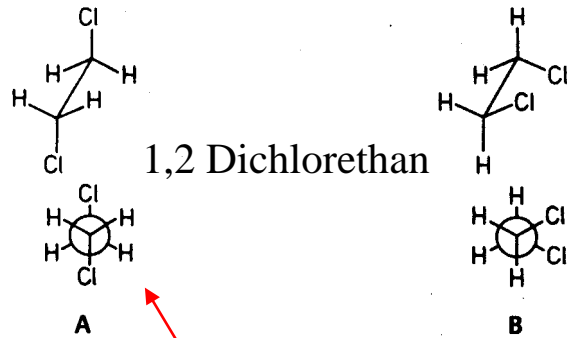
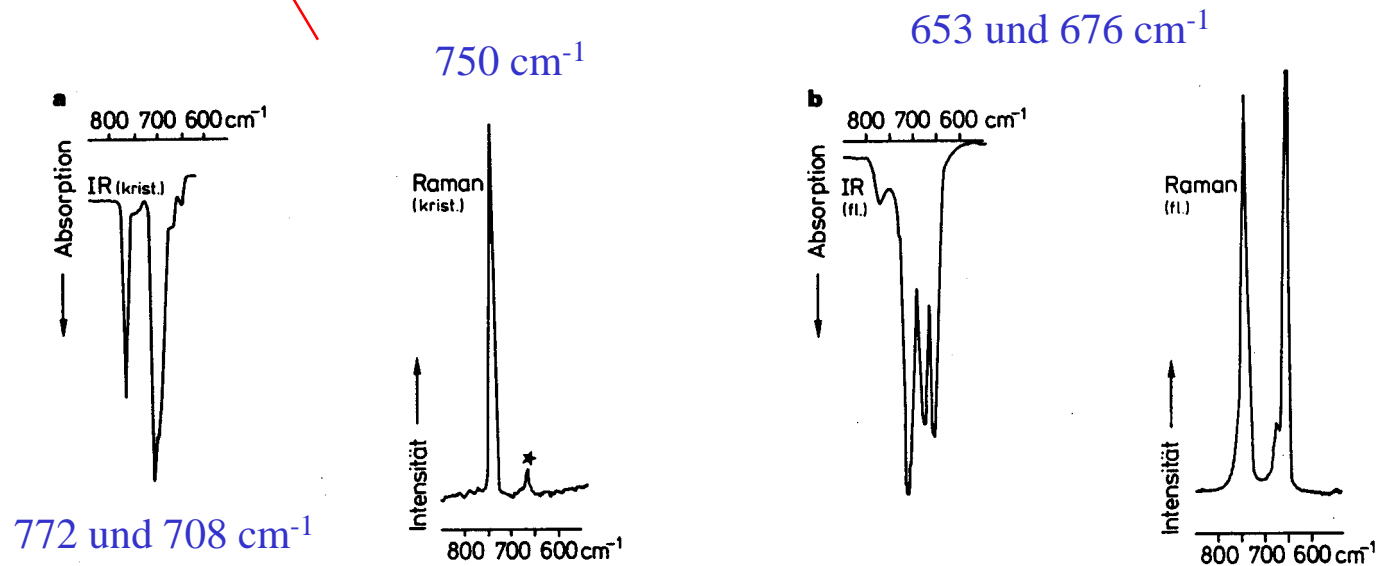


Abb. 14.11 1,2-Dichlorethan. A *trans*-, B *gauche*-Form

Rotationsisomerie:  
*trans*-Form A  
*gauche*-Form B

CCI-Valenzschwingung  
 600 bis 800  $\text{cm}^{-1}$

fest,  
 kristallin



# Beispiel: Dibenzanthrazene

Leicht polarisierbare  
Elektronensysteme:

$C\equiv C$ ,  $C=C$ ,  $C-C$

$C\equiv N$ ,

S-H,

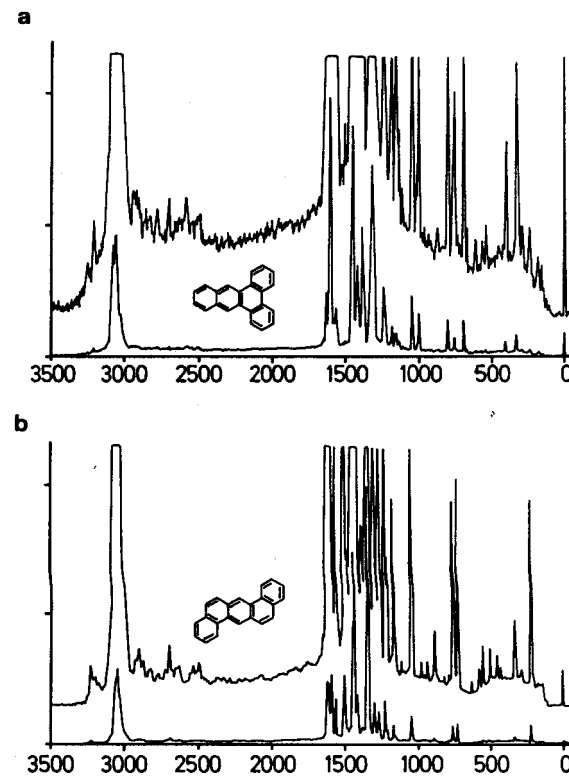
P-H,

C-S,

S-S,

Me-Me

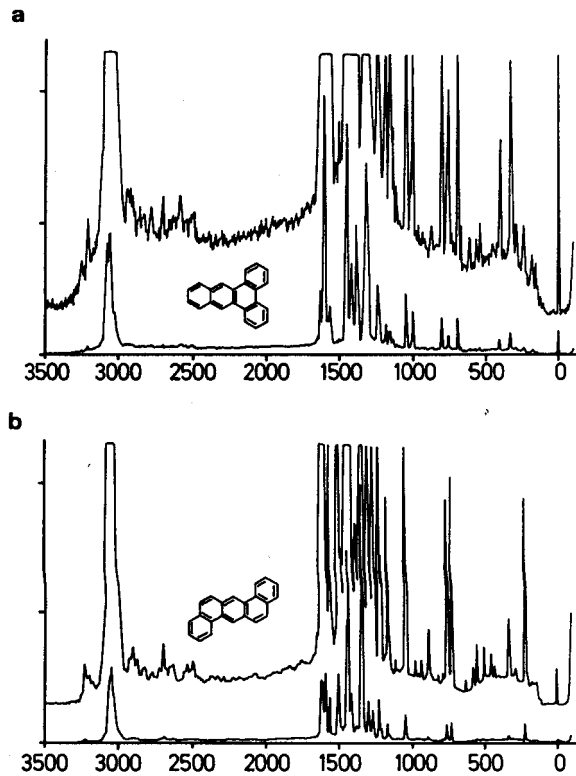
## Dibenzanthrazene



**Abb. 14.13** FT-Ramanspektren von PAH's<sup>17</sup>:  
**a** 1,2,3,4-Dibenzanthracen, **b** 1,2,5,6-Dibenzanthra-  
cen

# Beispiel: Autoabgase

## Dibenzanthrazene



## Gasanalytik

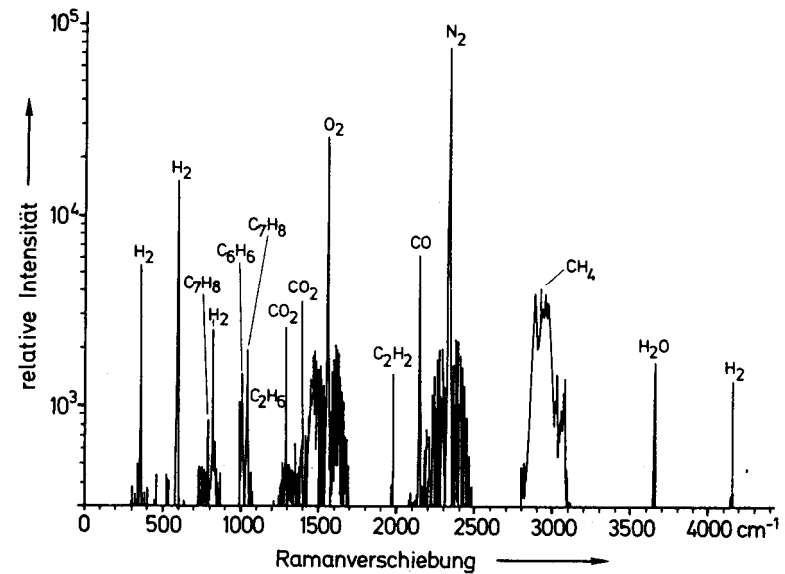
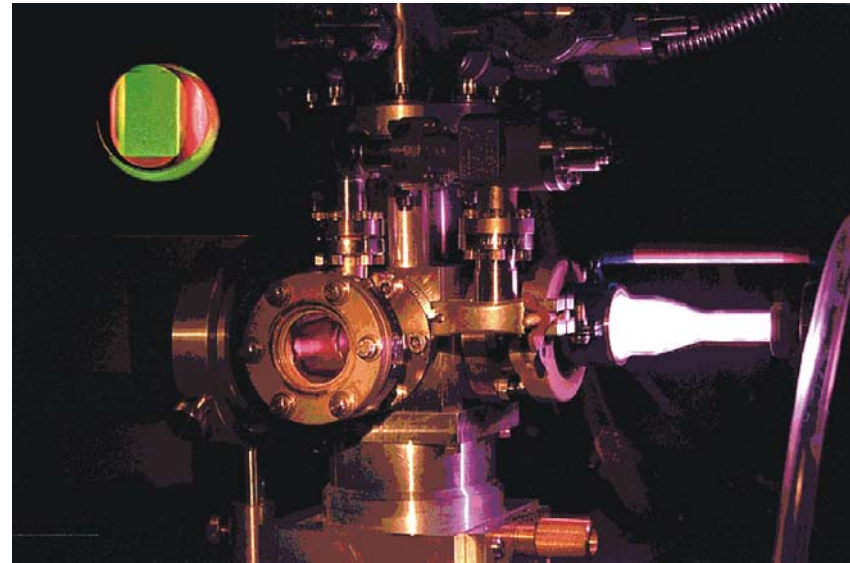
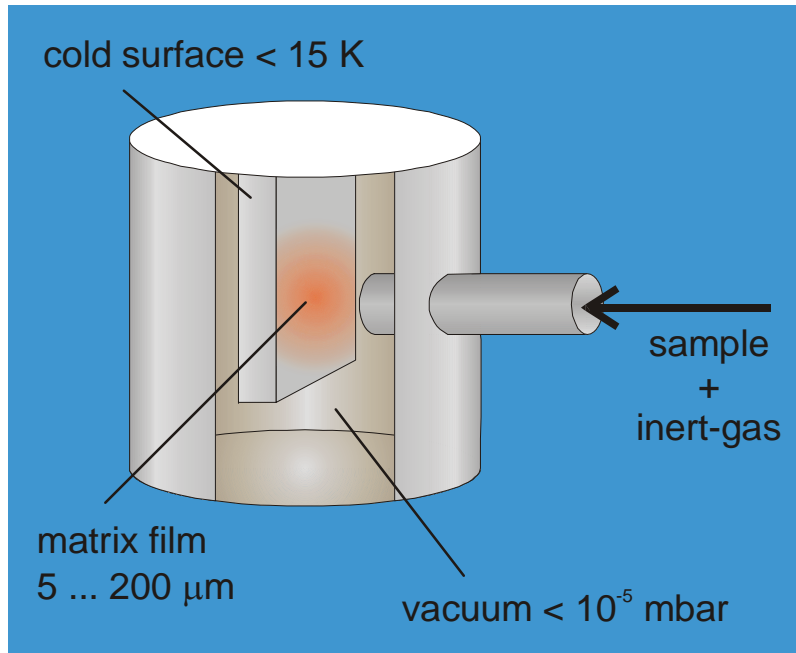


Abb. 14.13 FT-Ramanspektren von PAH's<sup>17</sup>:  
a 1,2,3,4-Dibenzanthracen, b 1,2,5,6-Dibenzanthra-  
cen

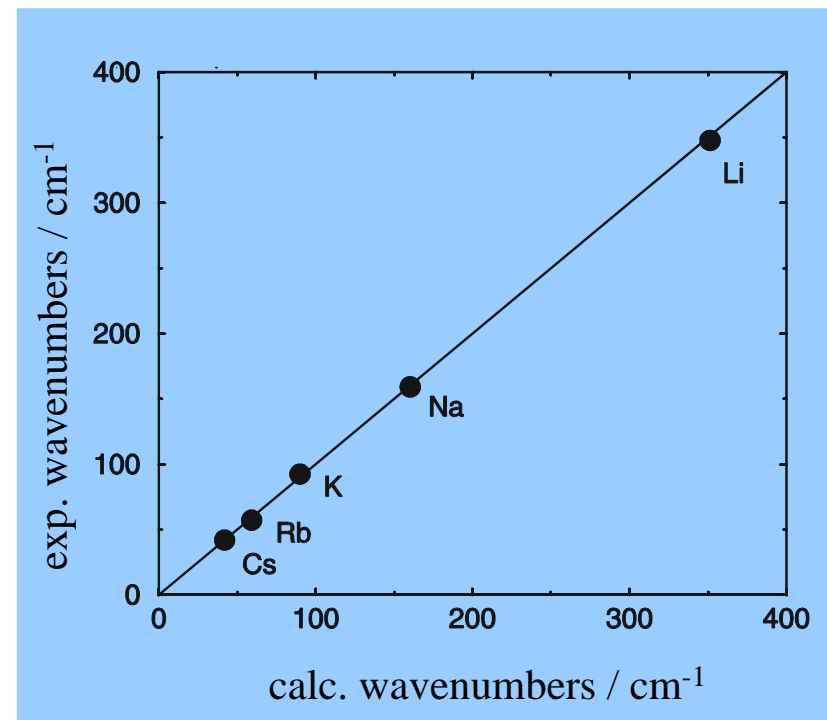
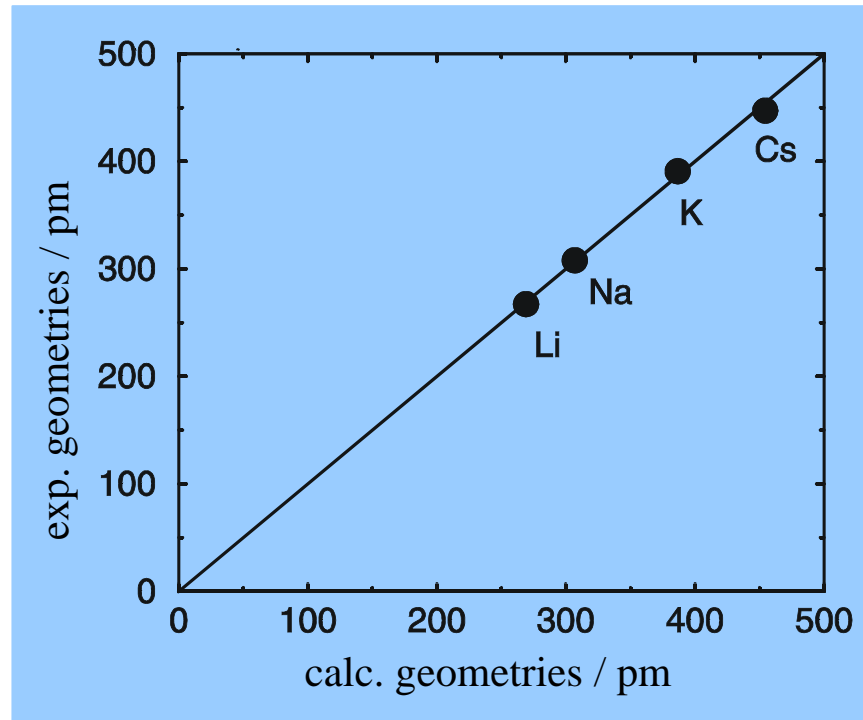
Wasserdampf?

# Beispiel: Atomare Cluster

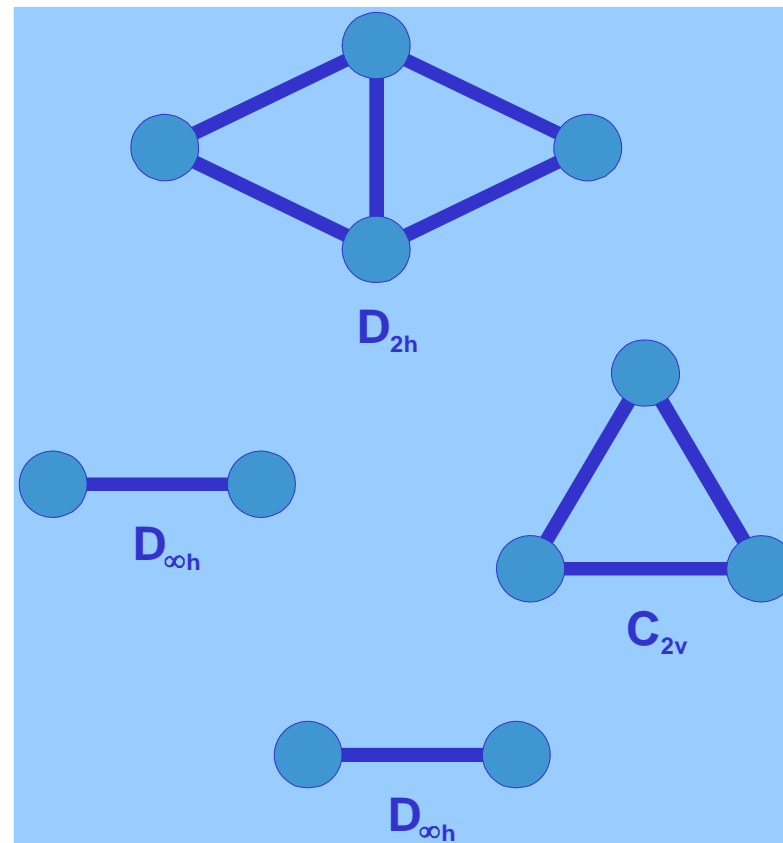
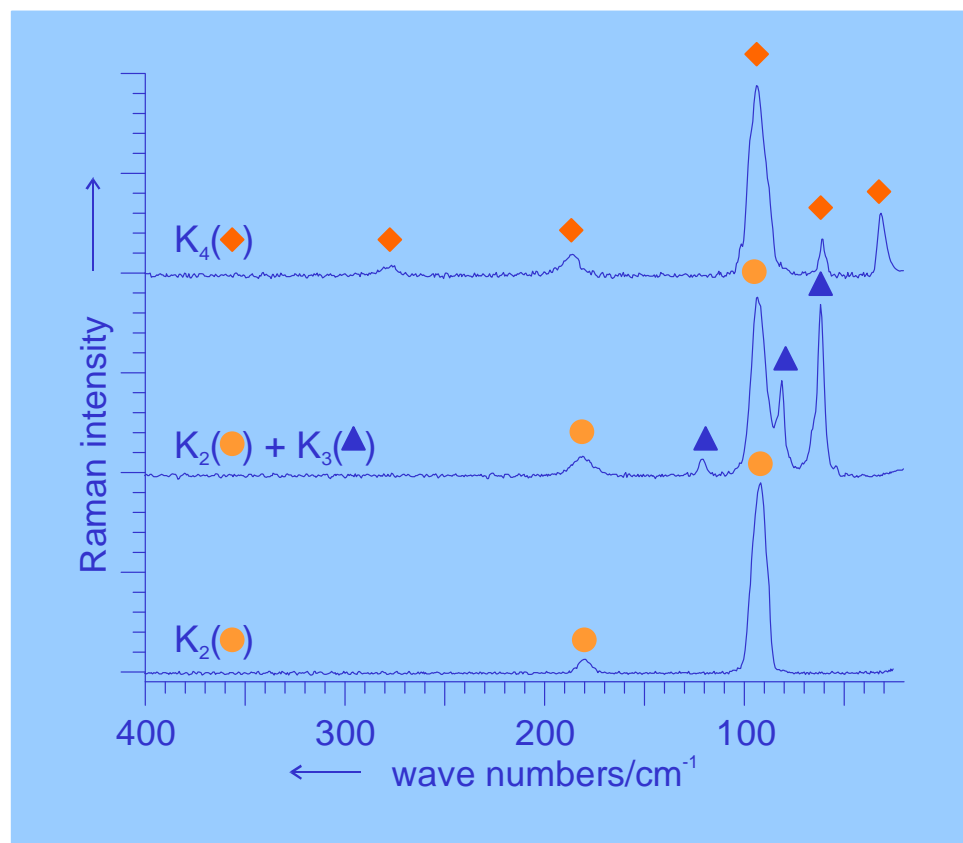


A. Kornath, R. Ludwig, A. Zoermer, *Angew. Chem. Int. Ed.*, 37, 1575-1577, 1998.

# Beispiele: Alkalidimer

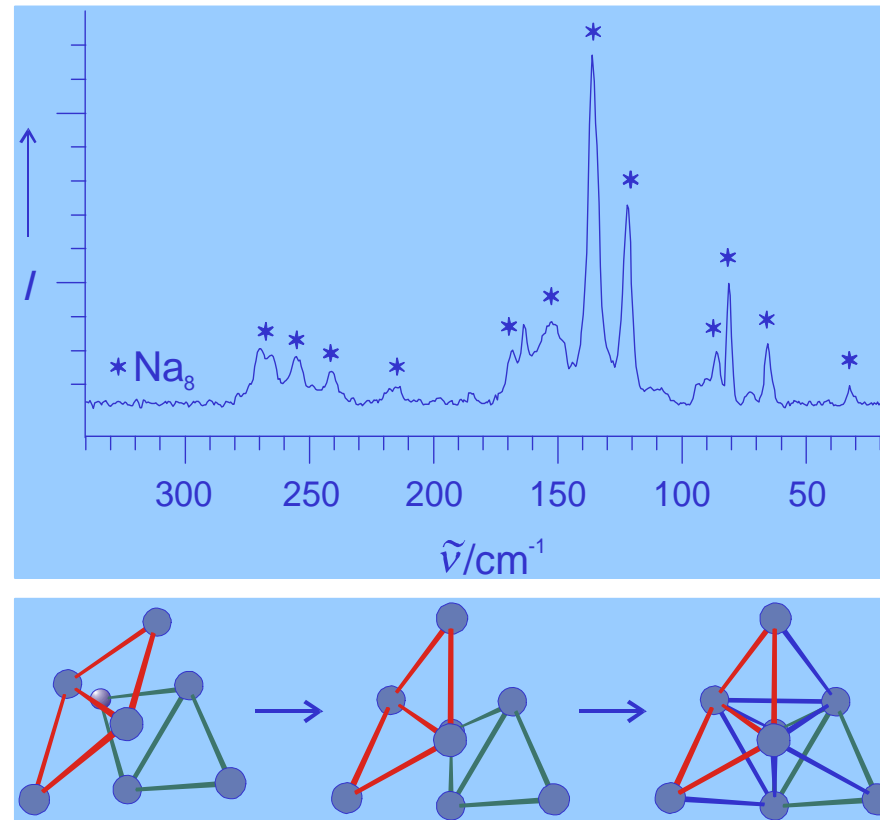


# Beispiele: Kaliumcluster



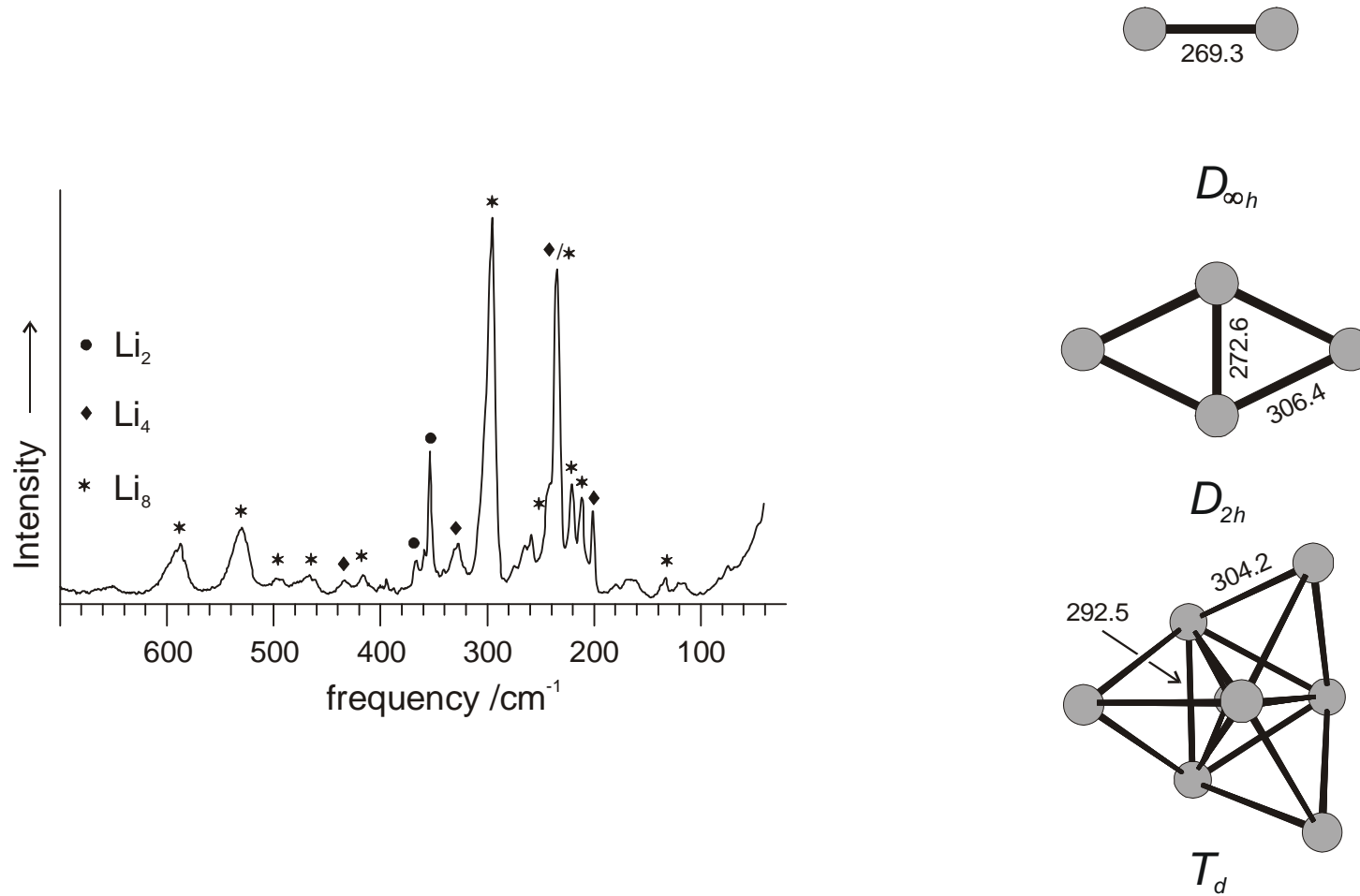
A. Kornath, R. Ludwig, A. Zoermer, *Angew. Chem. Int. Ed.*, 37, 1575-1577, 1998.

# Beispiel: Natriumcluster



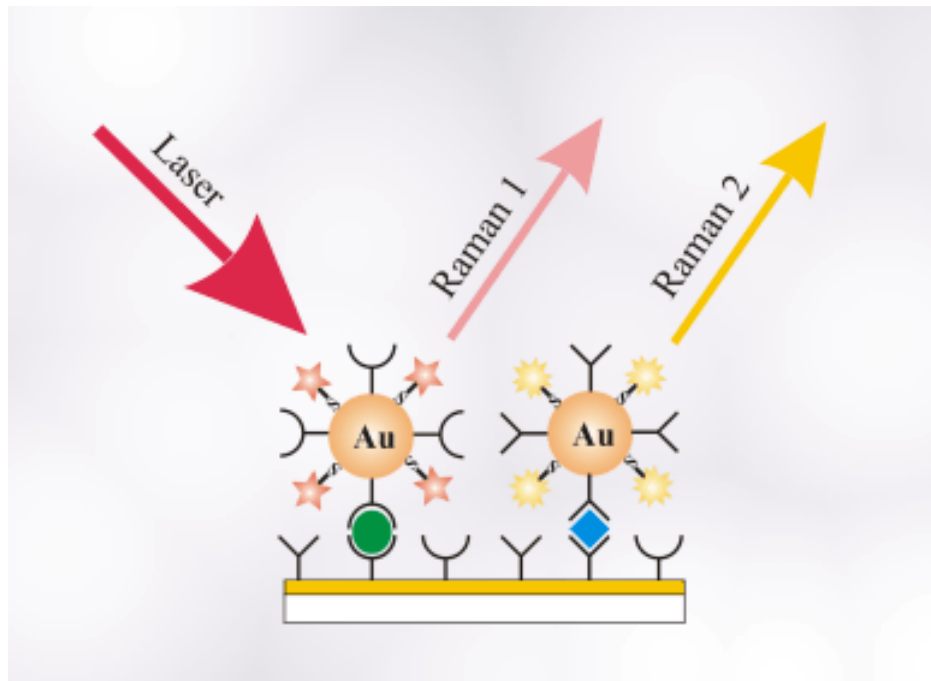
A. Kornath, R. Ludwig, A. Zoerner, *Inorg. Chem.*, 41, 6206-6210, 2002.

# Beispiel: Lithiumcluster



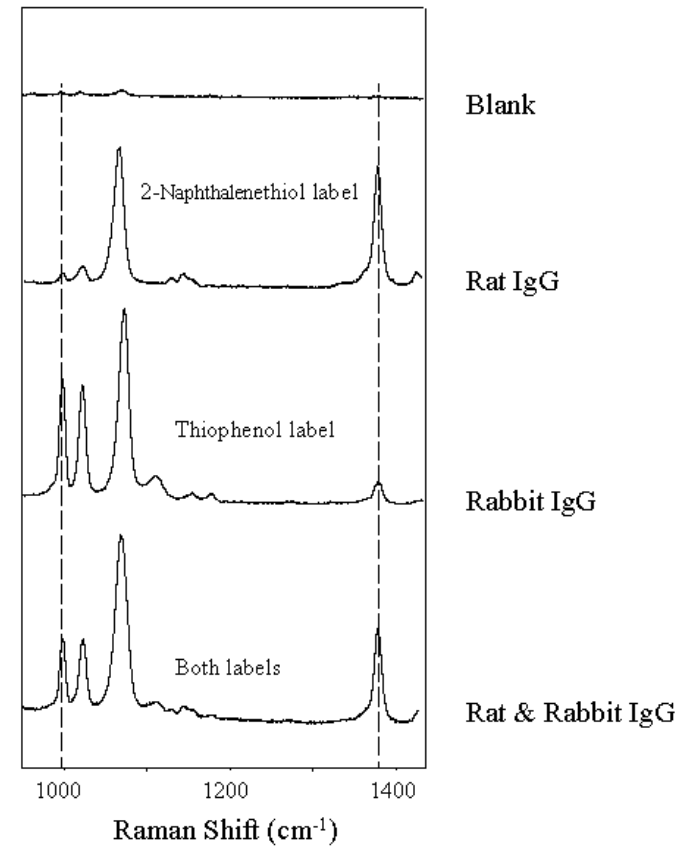
A. Kornath, R. Ludwig, A. Zoermer, J. Chem. Phys., im Druck.

# Beispiel: Biomoleküle

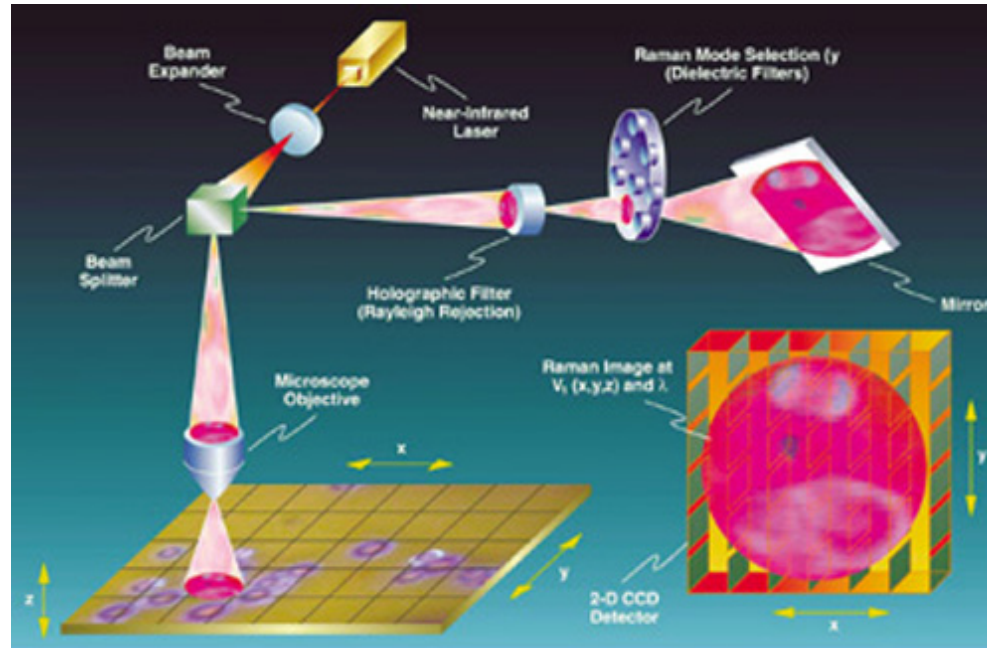


<http://www.mic.iastate.edu/instrumentation.html>

Simultaneous Detection of Rat & Rabbit IgG Using Surface Enhance Raman Spectroscopy

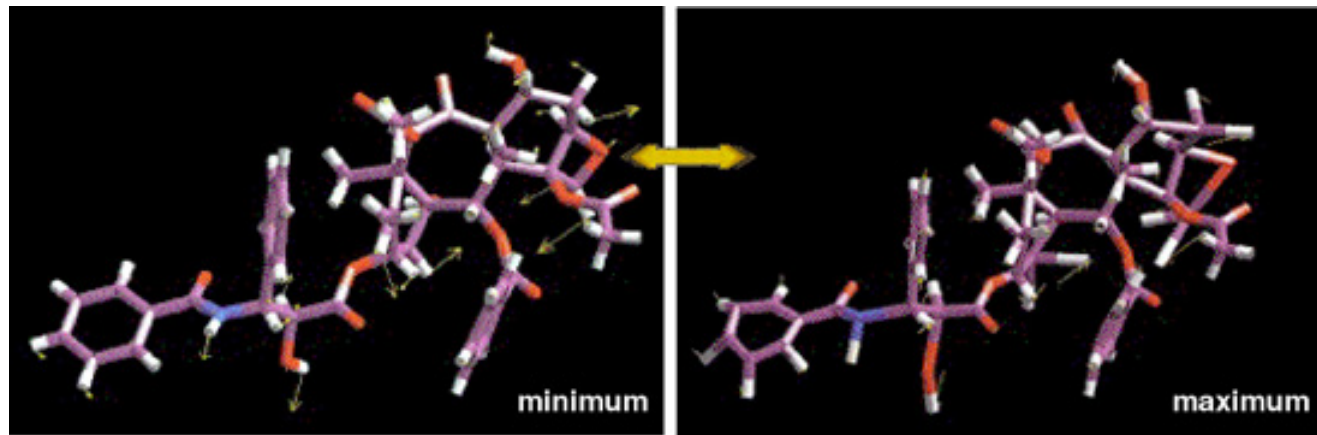


# Beispiel: Biomoleküle



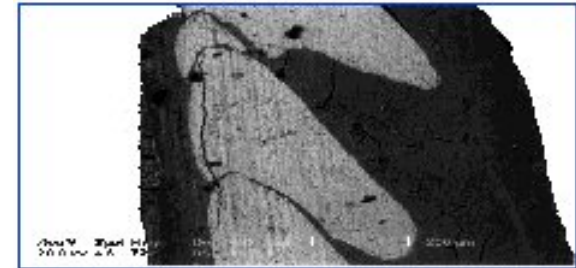
*In the global illumination instrumental arrangement used in modern Raman imaging, a beam of laser light is expanded and focused onto a target object, whereupon the Rayleigh component of light scattered back is rejected by a holographic filter. A specific Raman component is selected and the image that remains is projected onto a two-dimensional charged coupled device detector.*

# Beispiele: Biomoleküle



*The anti-cancer drug Taxol is shown undergoing a molecular vibration that appears at  $1,002\text{ cm}^{-1}$  in the Raman spectrum. Each frame shows the minimum and maximum displacements of molecular vibrations computed for this mode. Vectors indicate the atoms involved and the magnitude and direction of their motion. Computations at this level enable researchers to predict and correlate precisely structural variances in the molecule with the observed spectral features.*

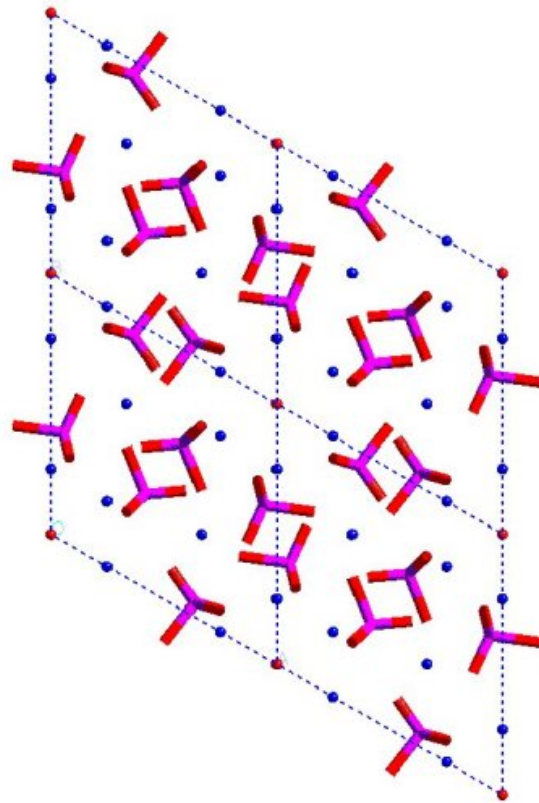
# Beispiele: Biomoleküle



Queen Parrotfish, *Scarus vetula*

[www.keele.ac.uk/depts/ch/groups/csg/caa/figure15\\_2.jpg](http://www.keele.ac.uk/depts/ch/groups/csg/caa/figure15_2.jpg)

# Beispiele: Biomoleküle



Four hydroxyapatite unit cells viewed down the c-axis. (00.1) face.

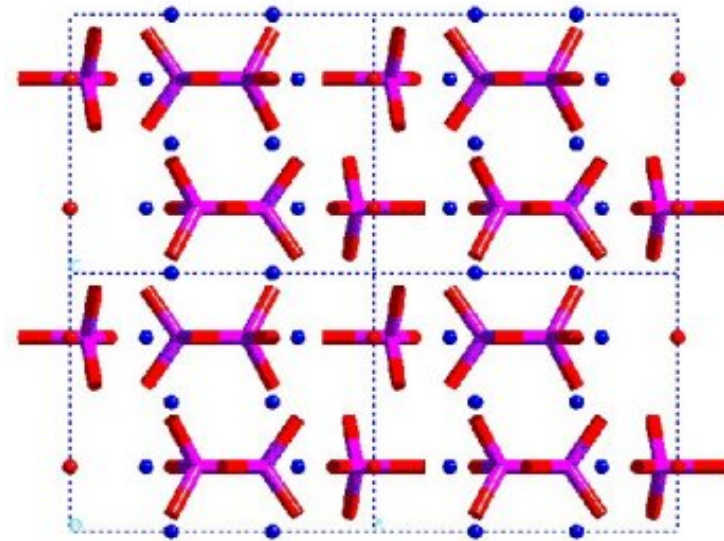
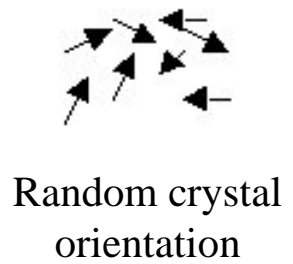
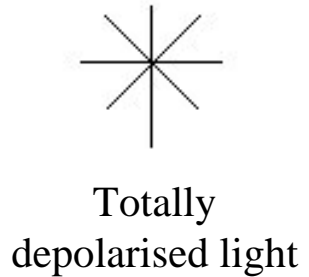


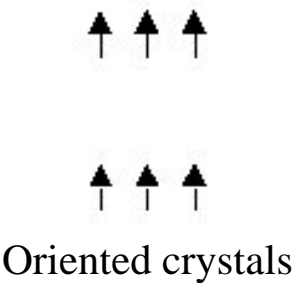
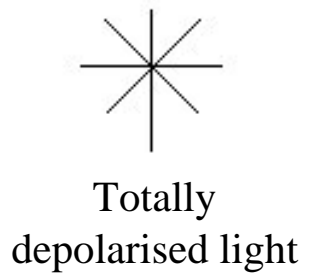
Figure 5. Four hydroxyapatite unit cells viewed down the a (or b) axis. (10.0) face.

# Beispiele: Biomoleküle

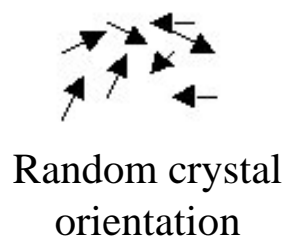
$$\rho = \frac{I_{\perp}}{I_{\parallel}}$$



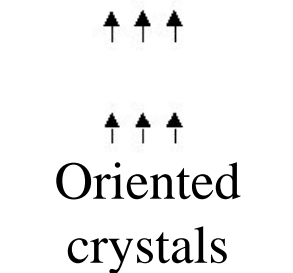
Raman Spectrum



Raman spectrum

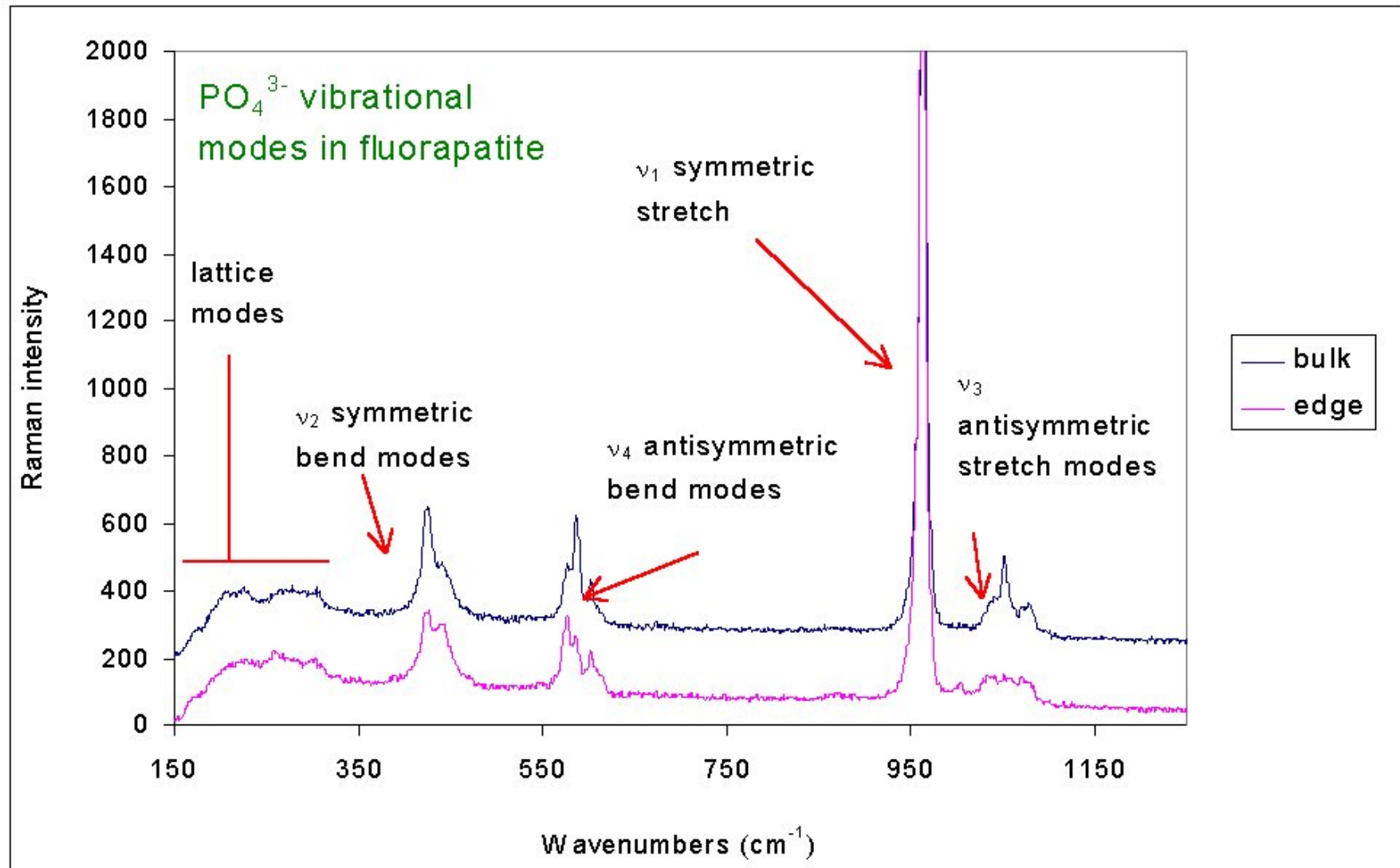


Raman spectrum with depolarisation ratios

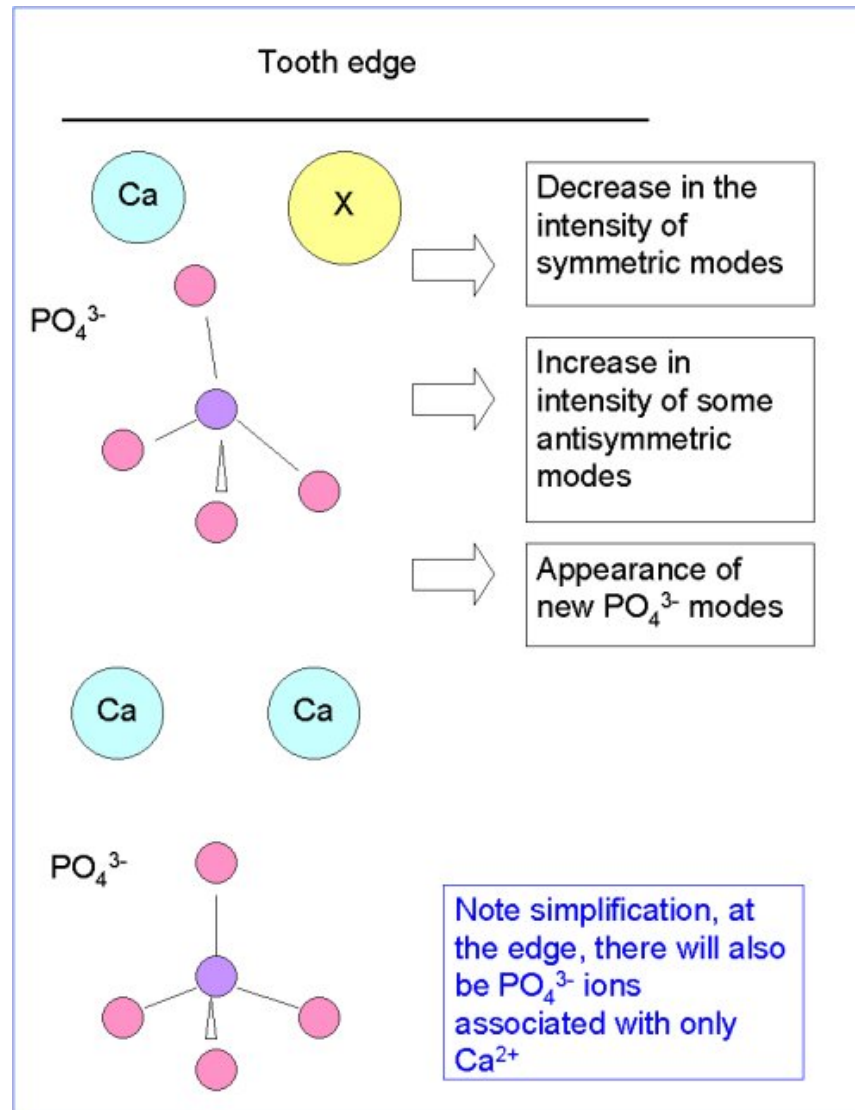


Polarised Raman spectrum

# Beispiele: Biomoleküle

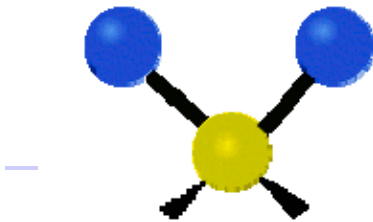


# Beispiele: Biomoleküle

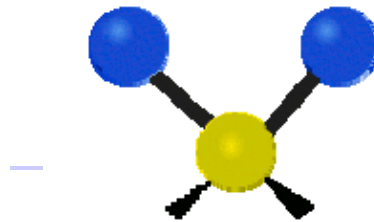


# Beispiele: Biomoleküle

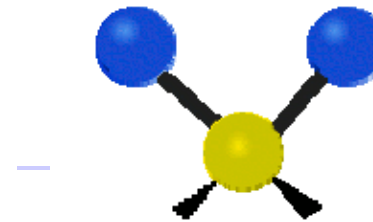
**Symmetrical stretching**



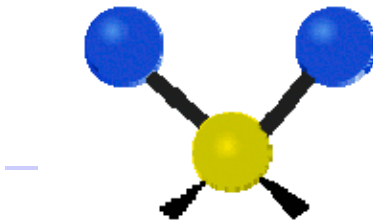
**Antisymmetrical stretching**



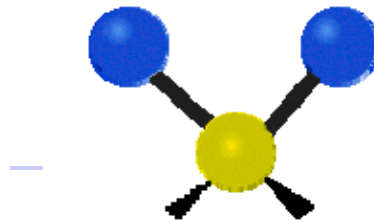
**Scissoring**



**Rocking**



**Wagging**



**Twisting**

