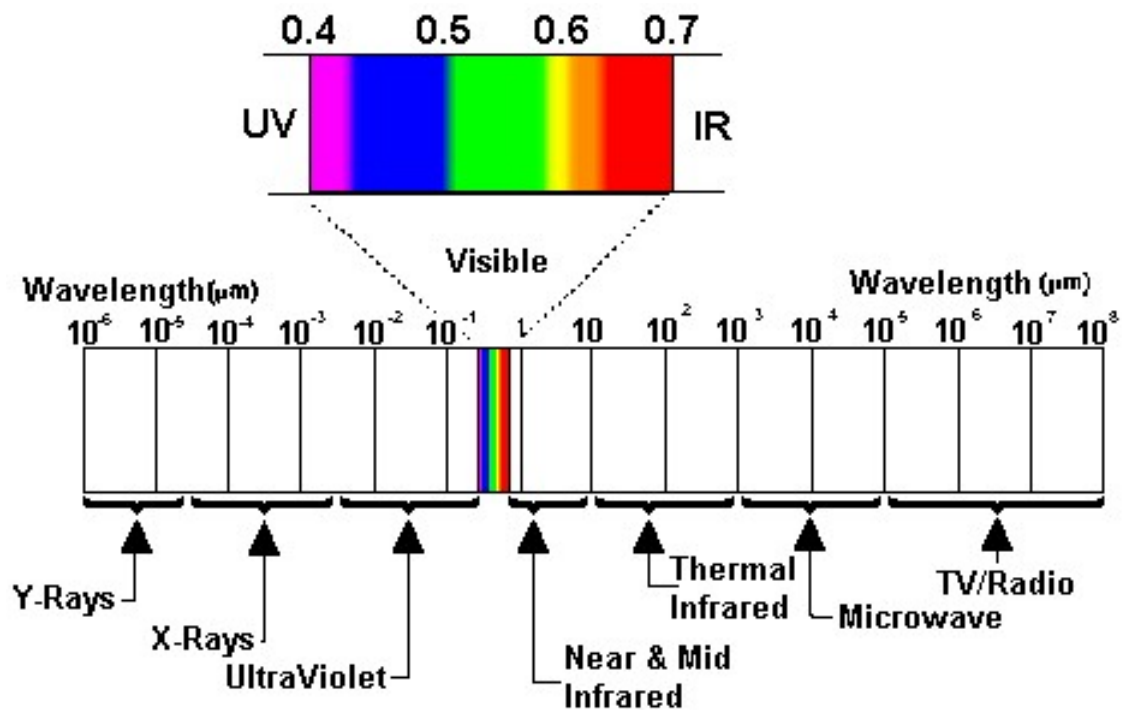


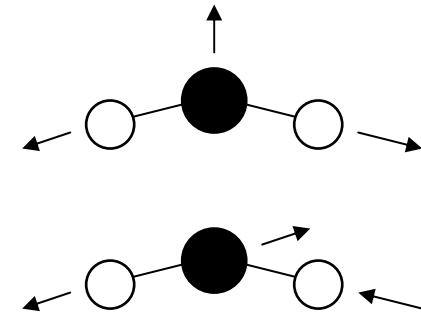
Infrarotspektroskopie



Spektralbereich	λ [μm]	ν [cm^{-1}]
NIR	0.8 bis 2.5	14.000 - 4.000
MIR	2,5 bis 50	4.000 - 800
FIR	50 bis 1000	800 - 40

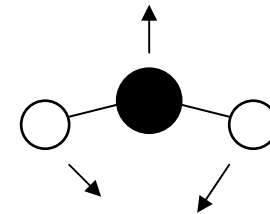
Typische Schwingungen

Valenzschwingungen: $\tilde{\nu}_s$ und $\tilde{\nu}_{as}$

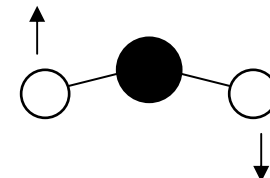


Deformationsschwingungen: δ und γ

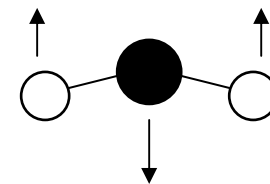
Biegeschwingung („Rocking“)



Torsionsschwingung („Twisting“)



Kippschwingung („Wagging“)

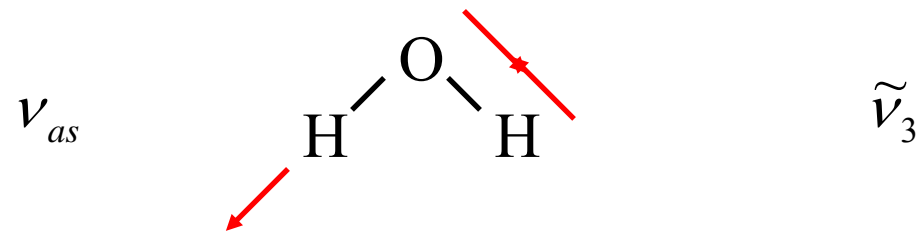
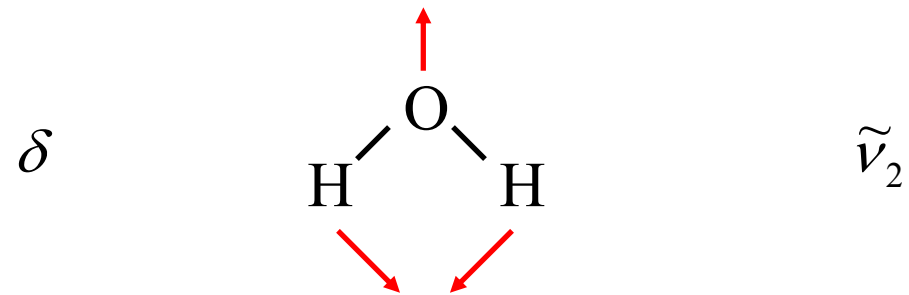
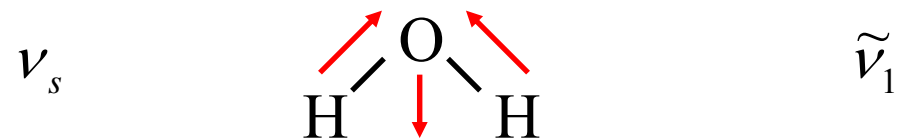


Normalschwingungen des CO₂-Moleküls

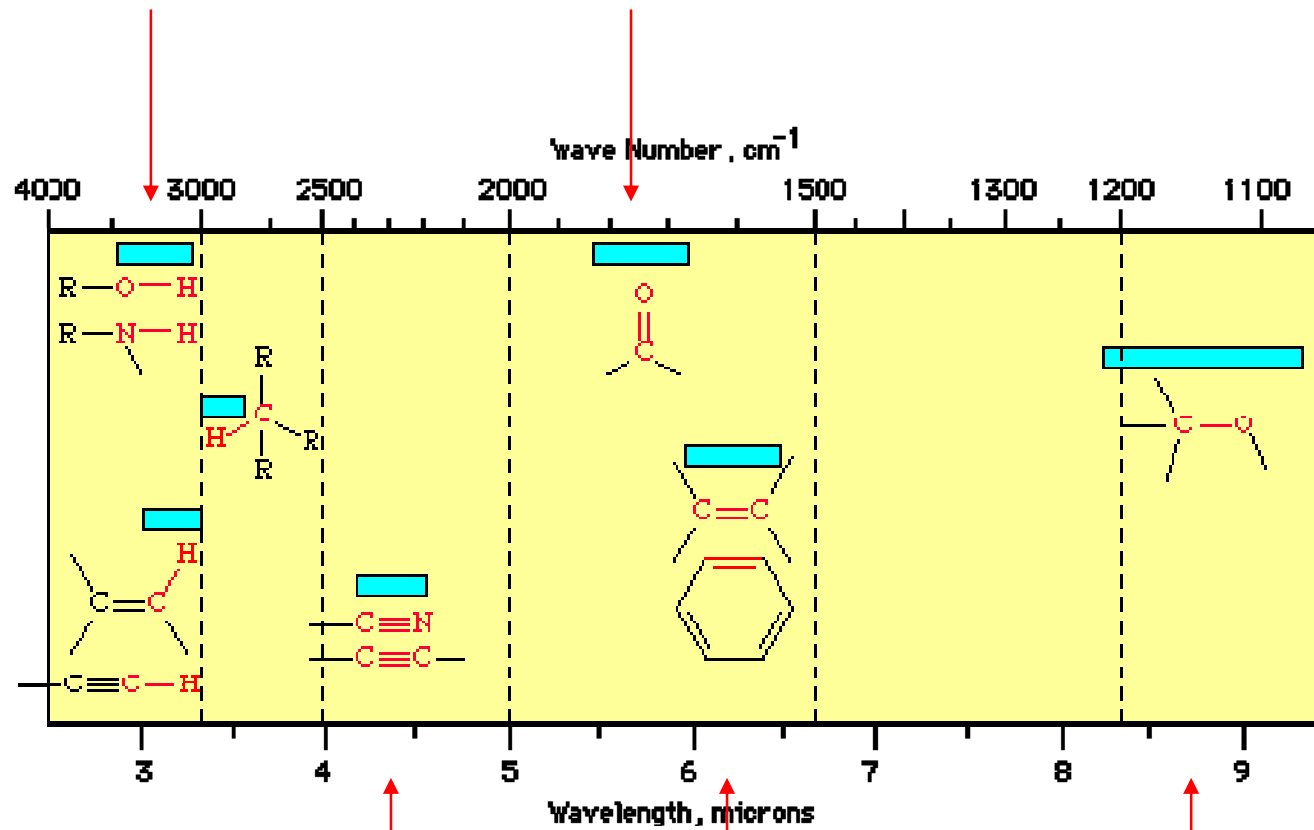
Zuordnung	Schwingungsform	Wellenzahl
ν_s	$\begin{array}{c} \rightarrow \qquad \rightarrow \\ O = C = O \end{array}$	$\tilde{\nu}_1$
ν_{as}	$\begin{array}{c} \rightarrow \quad \leftarrow \quad \rightarrow \\ O = C = O \end{array}$	$\tilde{\nu}_2$
δ	$\begin{array}{c} \uparrow \qquad \qquad \uparrow \\ O = C = O \\ \downarrow \end{array}$	$\tilde{\nu}_3 = \tilde{\nu}_4$
δ	$\begin{array}{c} + \quad - \quad + \\ O = C = O \end{array}$	$\tilde{\nu}_3 = \tilde{\nu}_4$

Normalschwingungen des H₂O-Moleküls

Zuordnung Schwingungsform Wellenzahl



Gruppenfrequenz

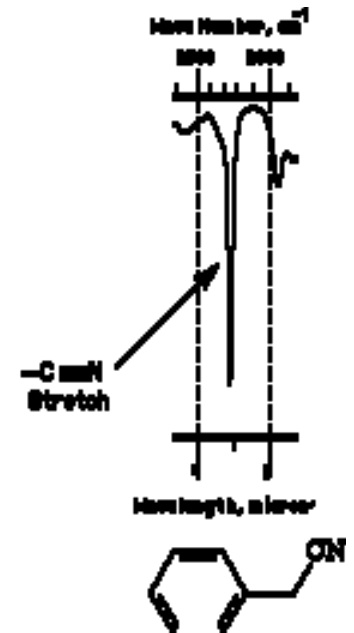
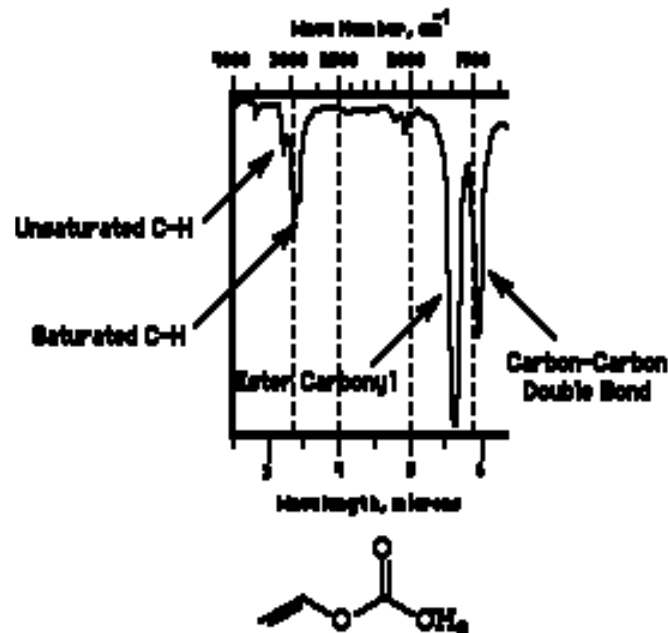
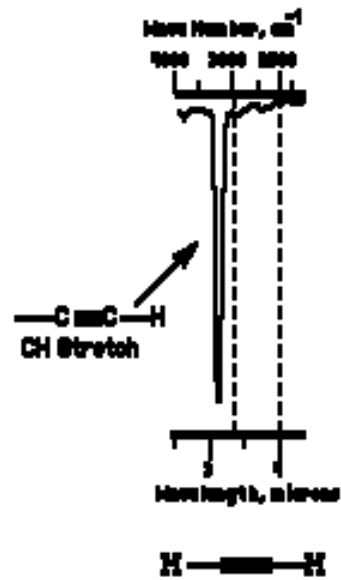
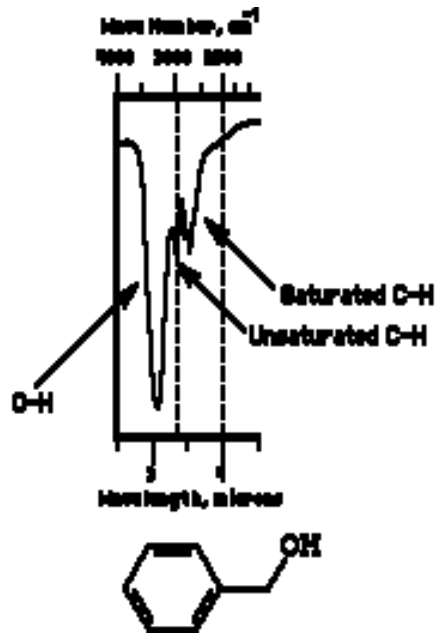


dreifach

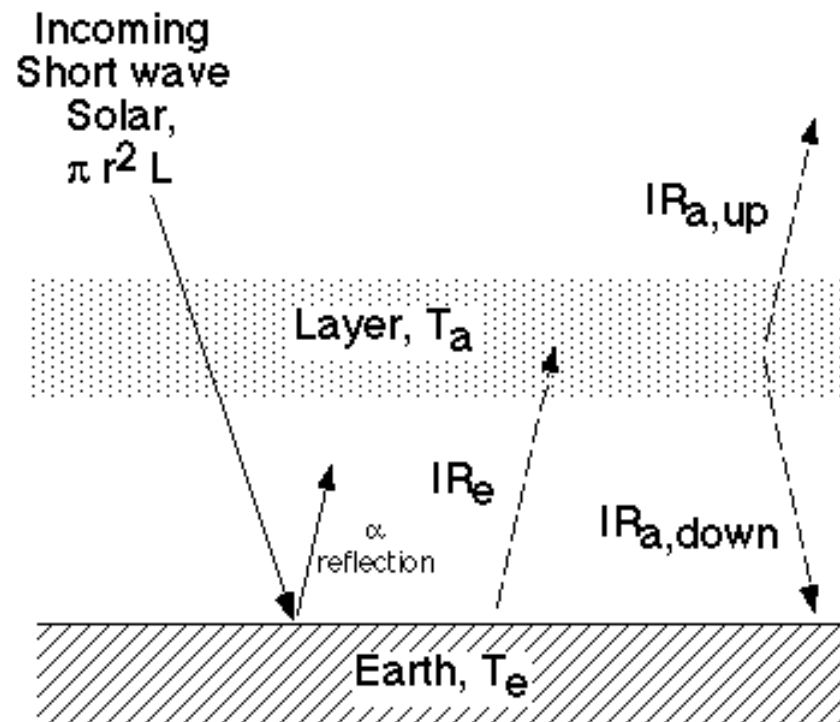
zweifach

einfach

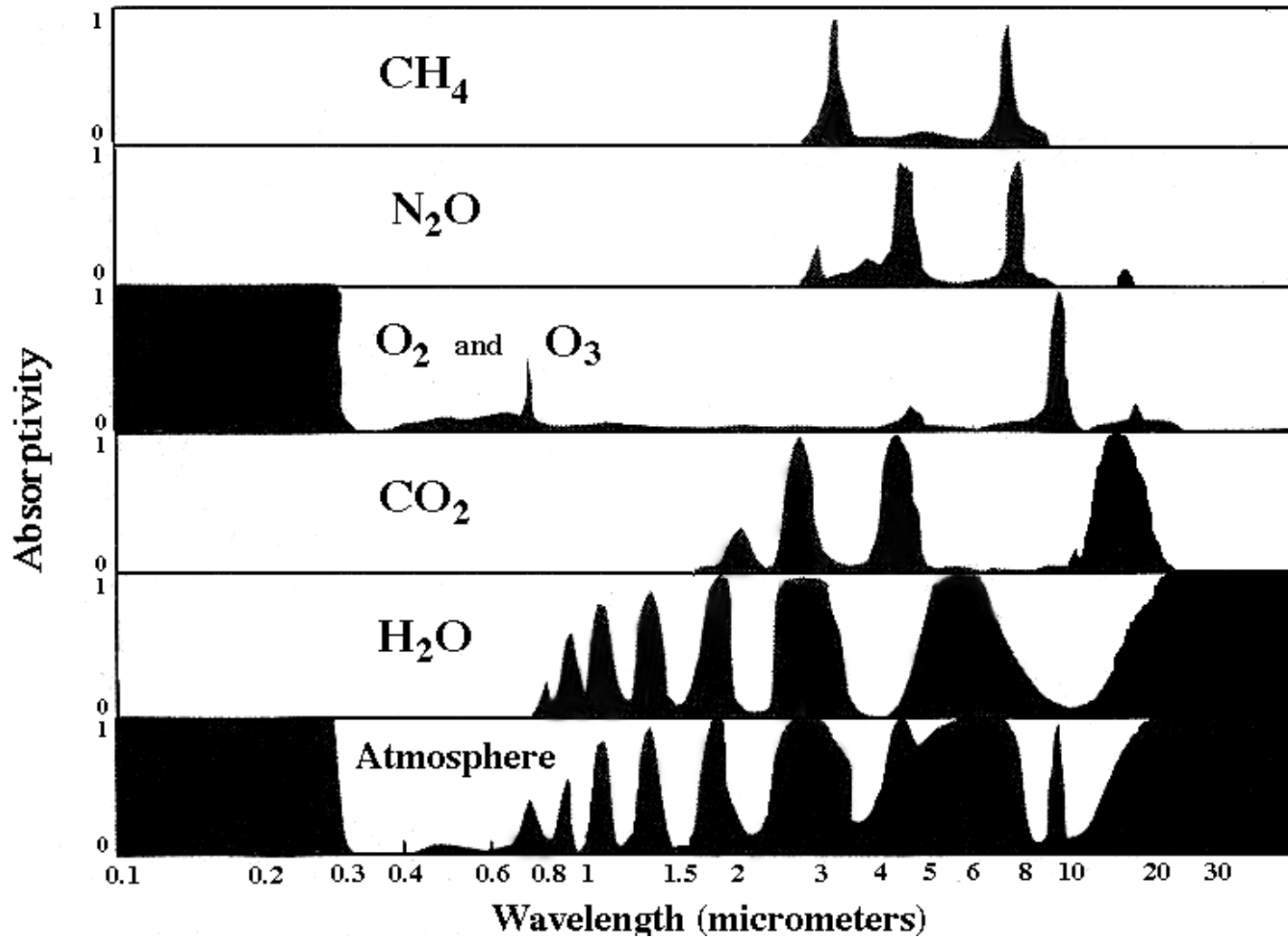
IR-Spektrum



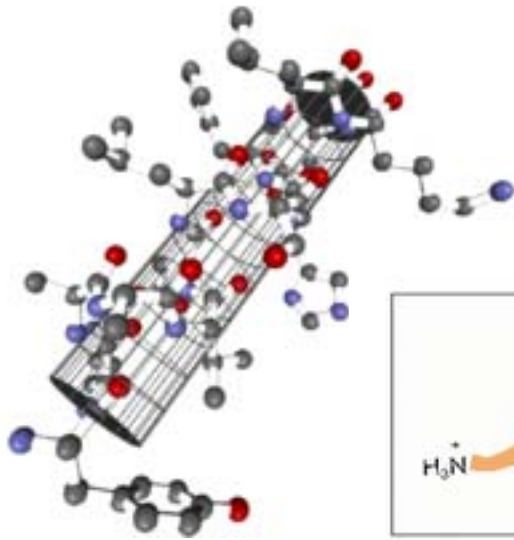
Beispiel 1. Atmosphäre



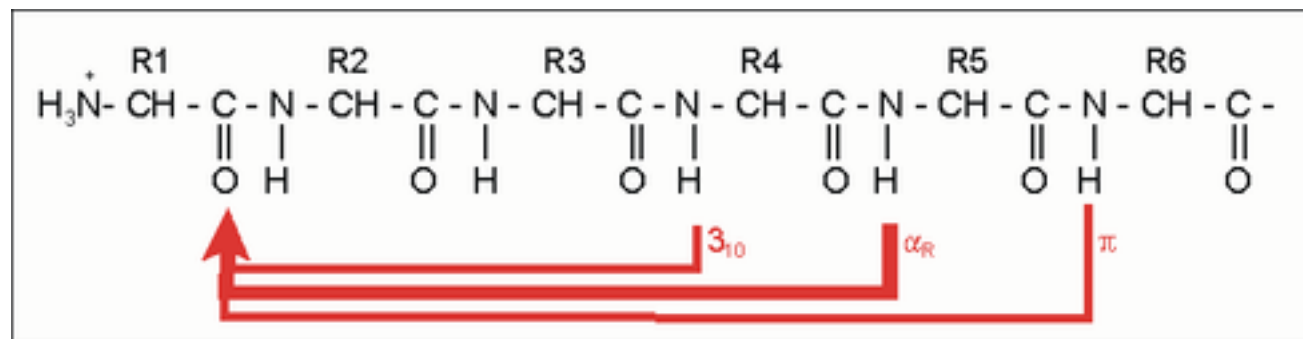
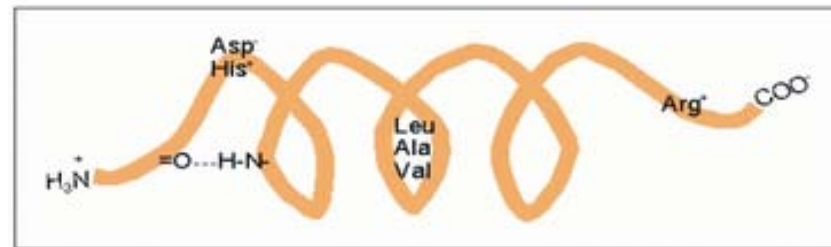
Beispiel 1: Atmosphäre



Beispiel 2: Sekundärstrukturelemente

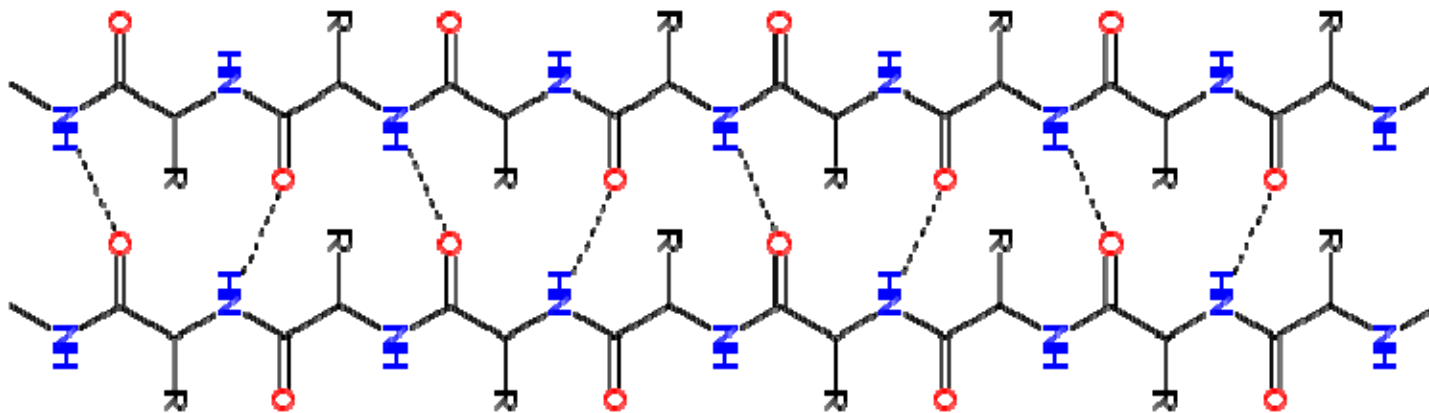
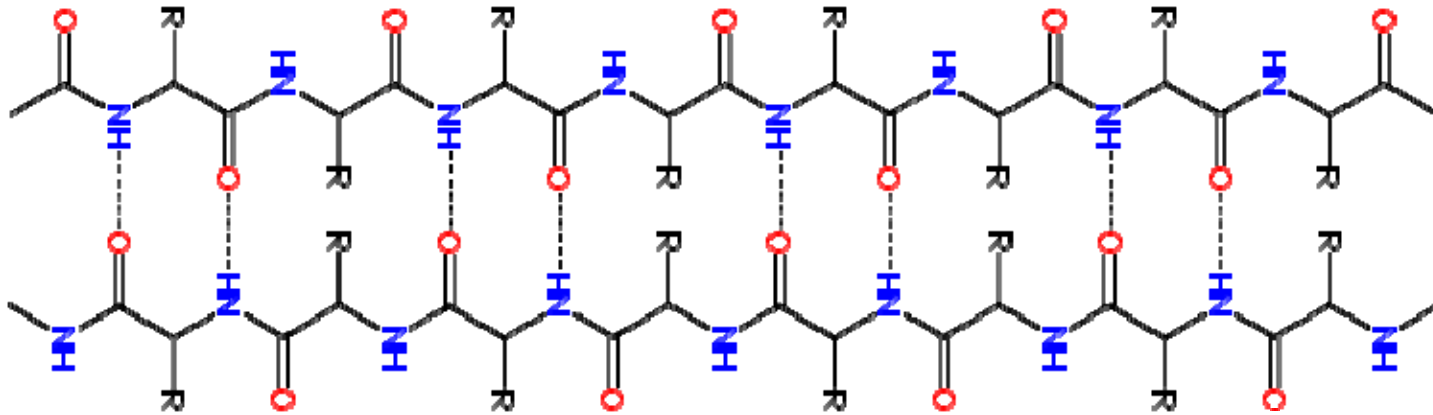


Helices

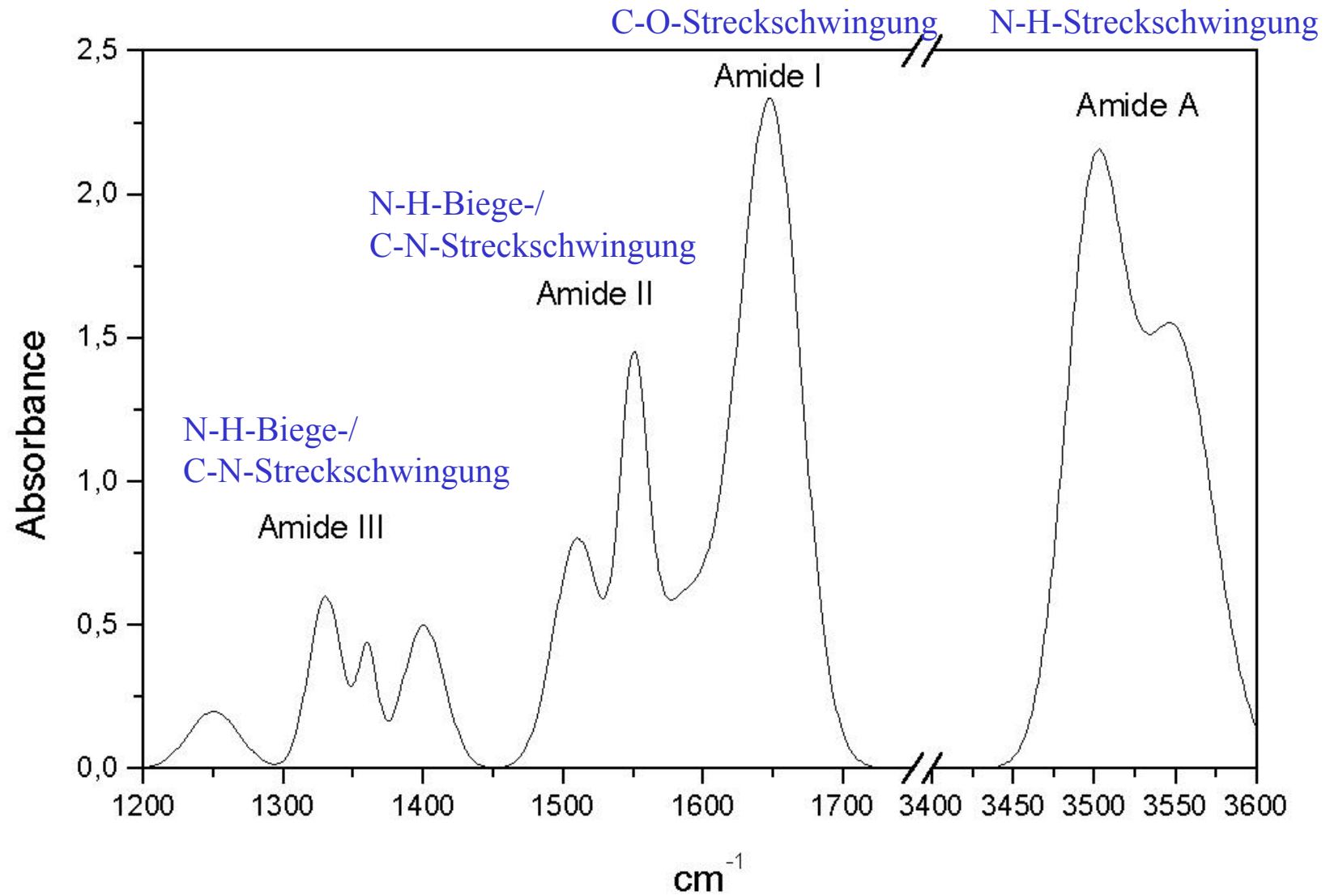


Beispiel 2: Sekundärstrukturelemente

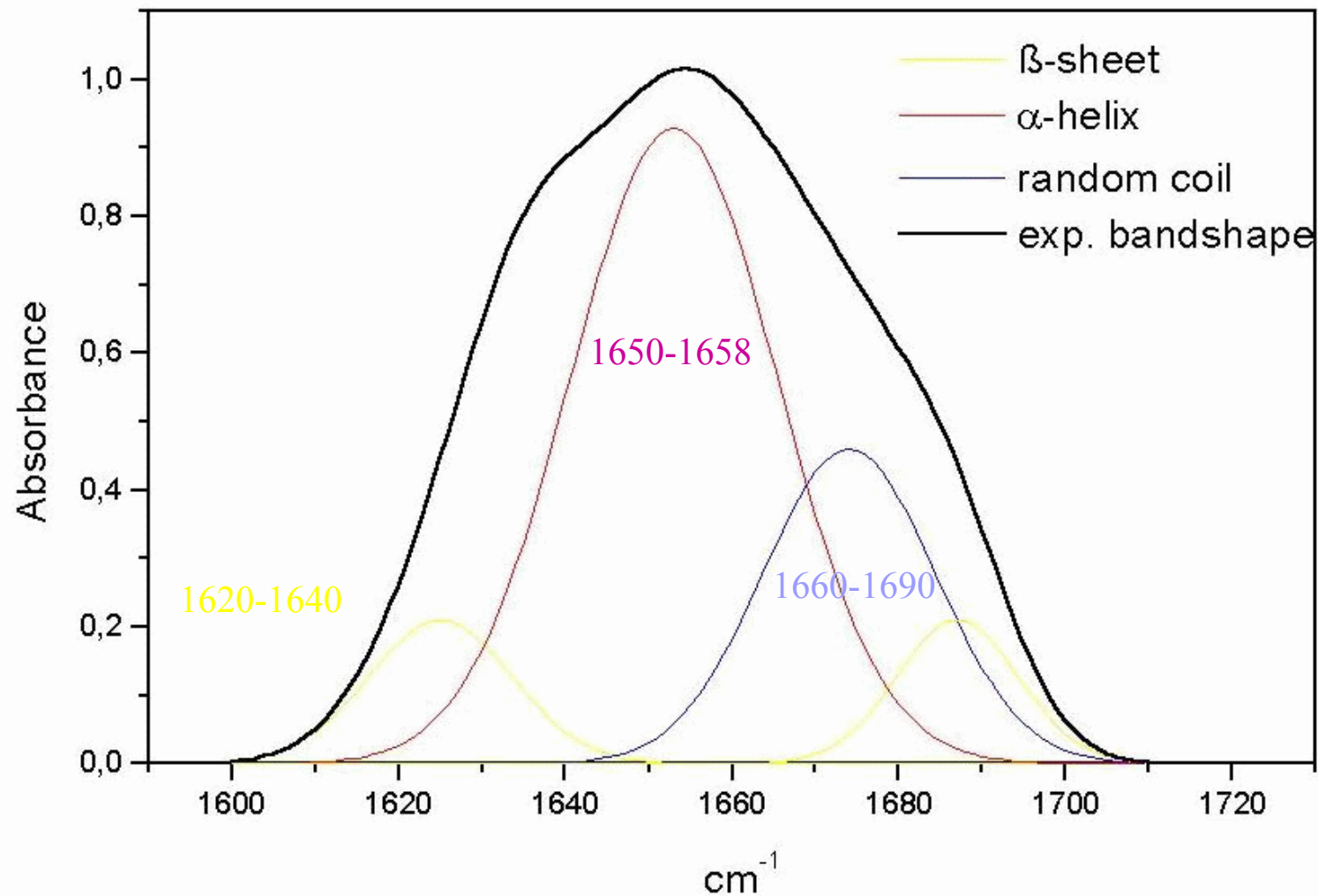
β -sheets



Beispiel 2: Proteine



Beispiel 2: Proteine

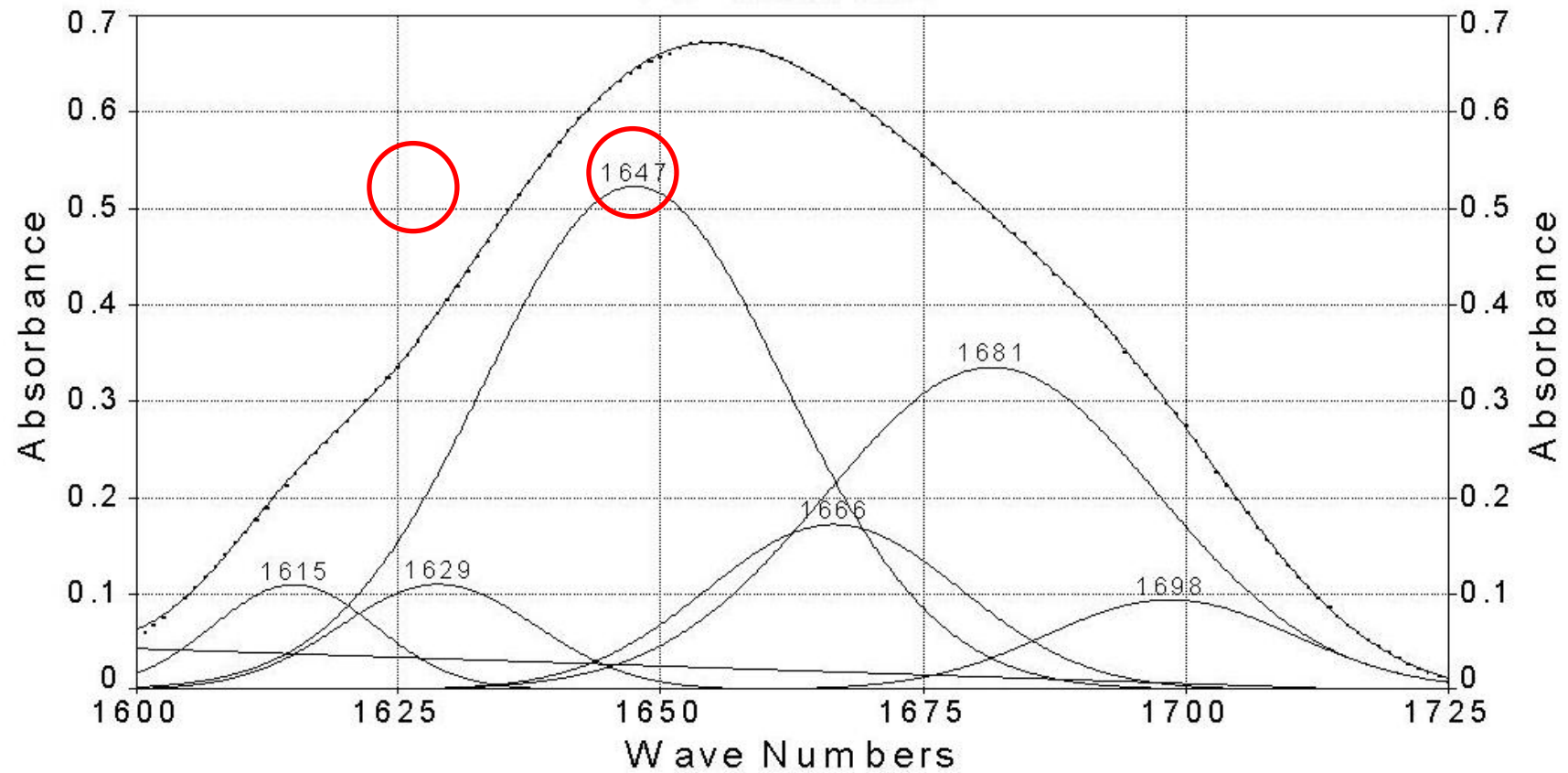


Beispiel 2: Proteine

Lysozyme

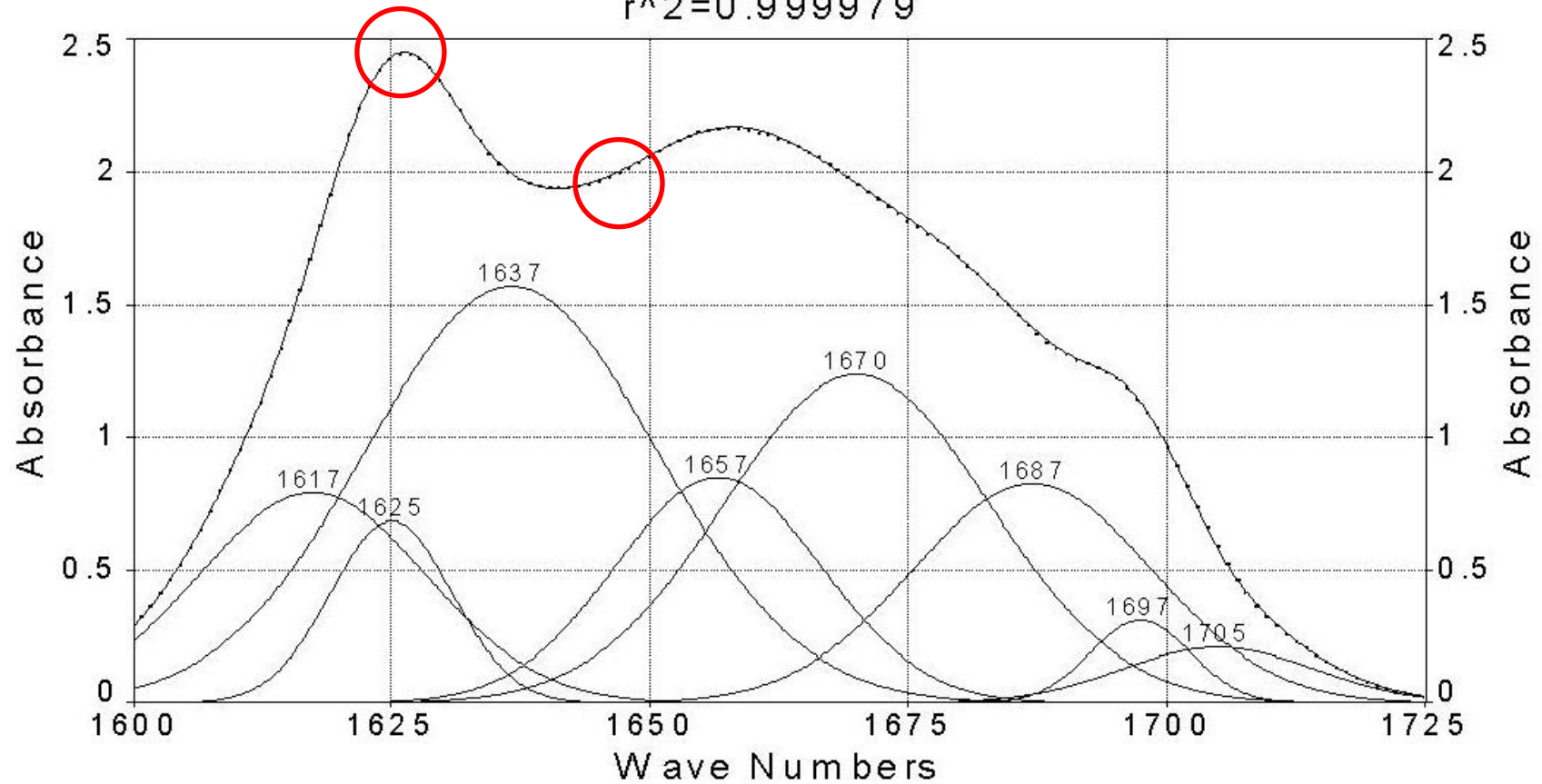
Gauss 6 Peaks

$r^2=0.999962$



Beispiel 2: Proteine

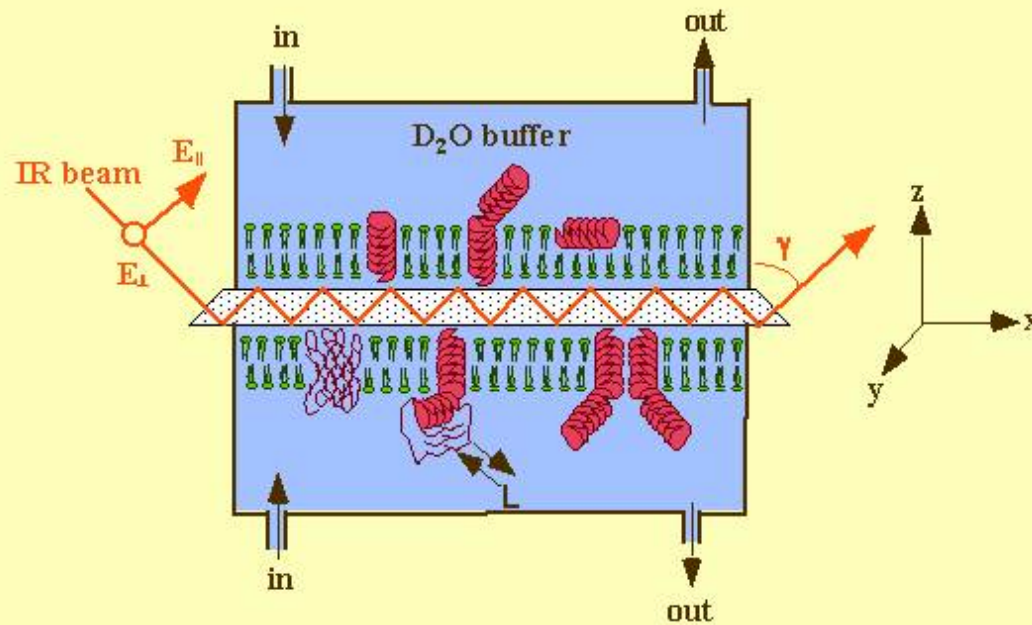
Lysozyme den.
Gauss 8 Peaks
 $r^2=0.999979$



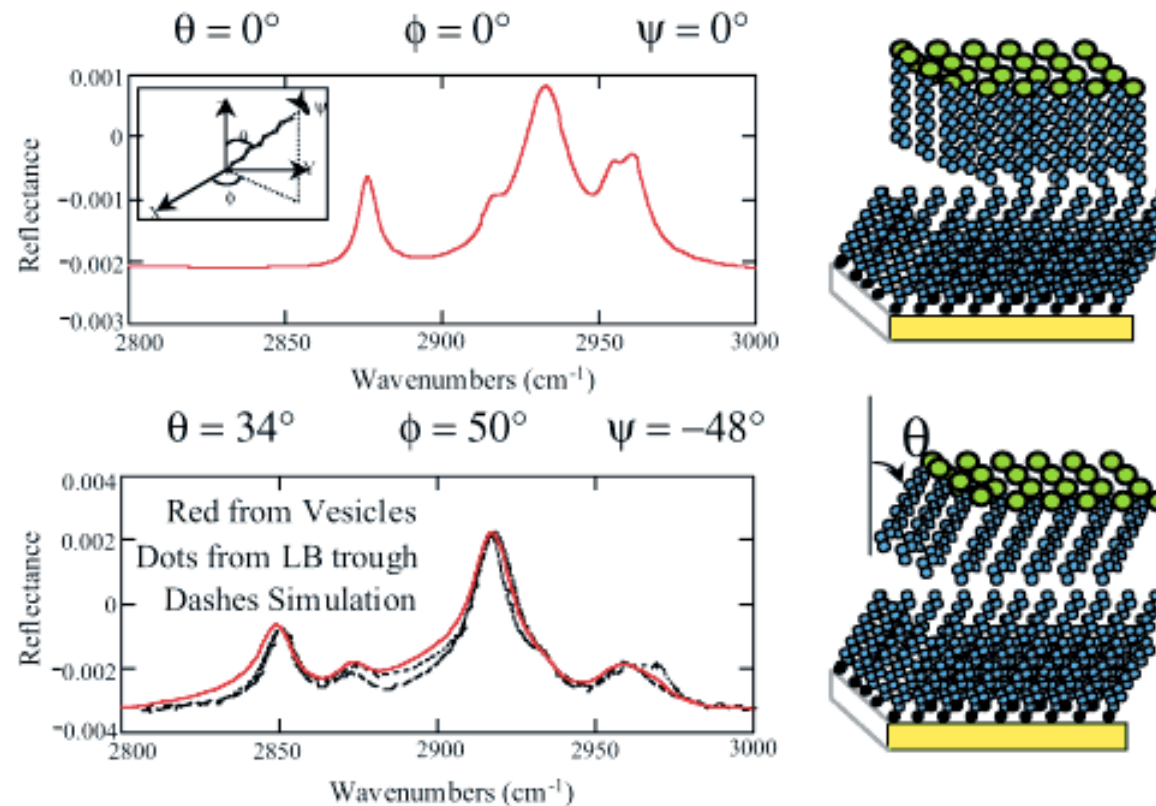
Beispiel 2: Proteine

ATR - FTIR Spectroscopy

to determine secondary structure, orientation, conformational and dynamic changes in membrane proteins



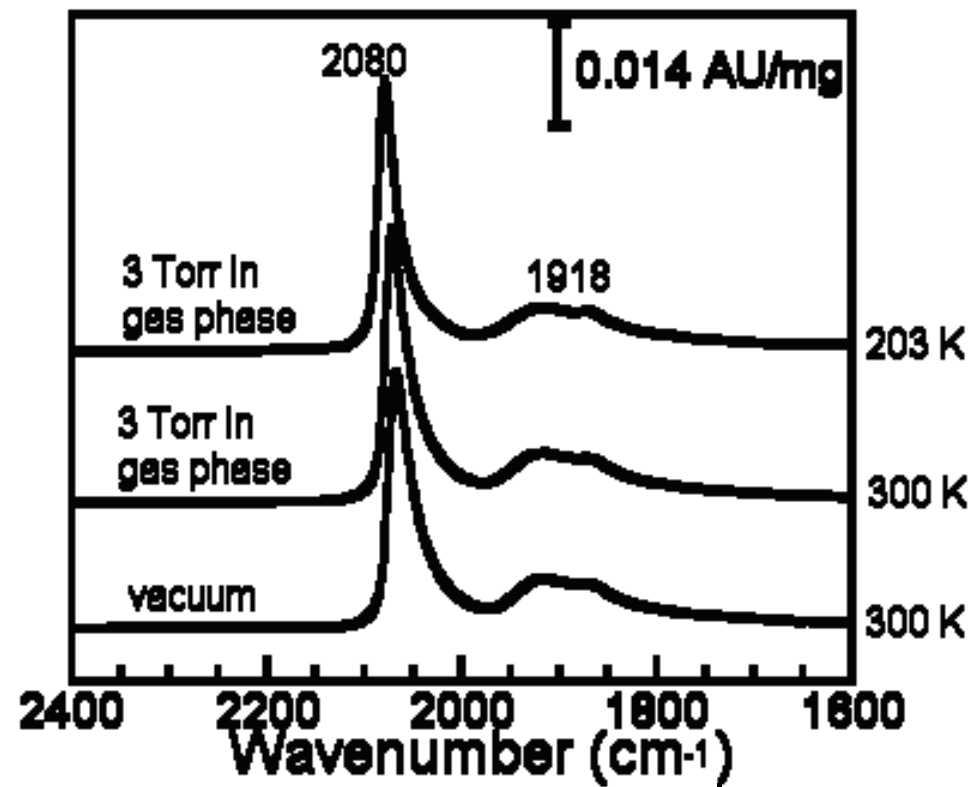
Beispiel 3: Lipide



C. W. Meuse, S. Kruegar, C. F. Majkrzak, J. A. Dura, J. Fu., J. T. Connor, A. L. Plant "Hybrid Bilayer Membranes in Air and Water: Infrared Spectroscopy and Neutron Reflectivity Studies," *Biophys. J.* 1998, 74, 1388.

Beispiel 4: Oberflächen

FTIR of CO on Rh/SiO₂



Beispiel 4: Oberflächen

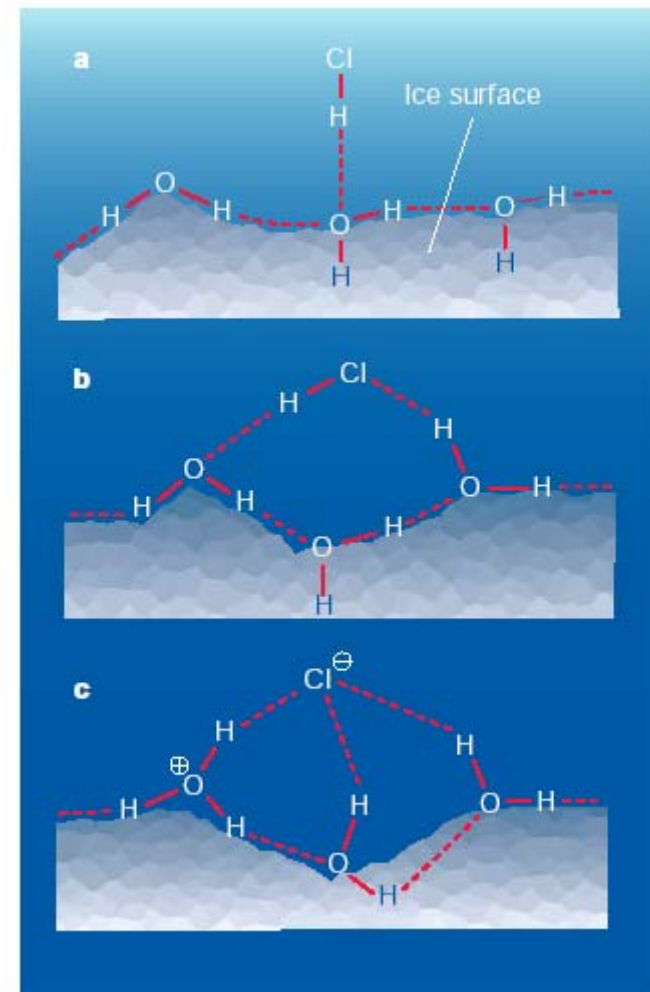
Discrete stages in the solvation and ionization of hydrogen chloride adsorbed on ice particles

J. P. Devlin*, N. Uras*, J. Sadlej† & V. Buch‡

* Department of Chemistry, Oklahoma State University, Stillwater, Oklahoma 74078, USA

† Department of Chemistry, University of Warsaw, Pasteura 1, 02-093 Warsaw, and Drug Institute, 00-725 Warsaw, Poland

‡ Fritz Haber Institute for Molecular Dynamics, Hebrew University, Jerusalem, Israel 91904



Beispiel 4: Oberflächen

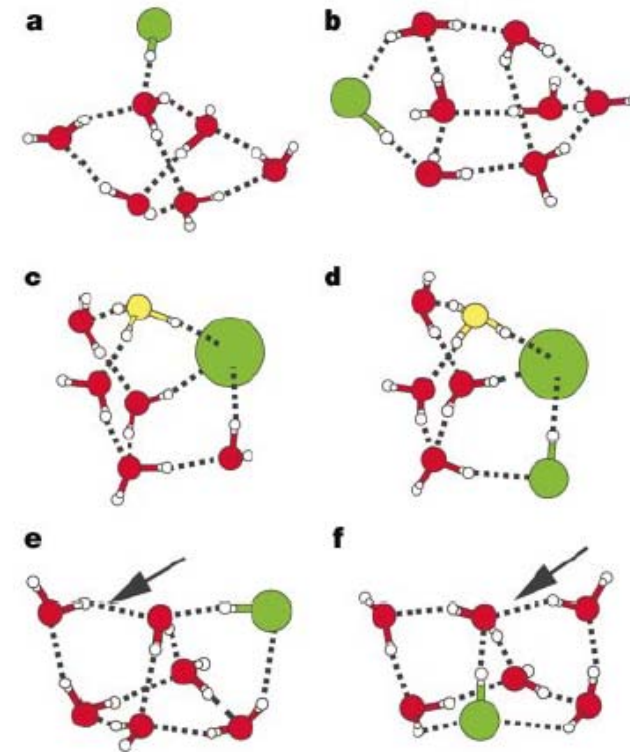
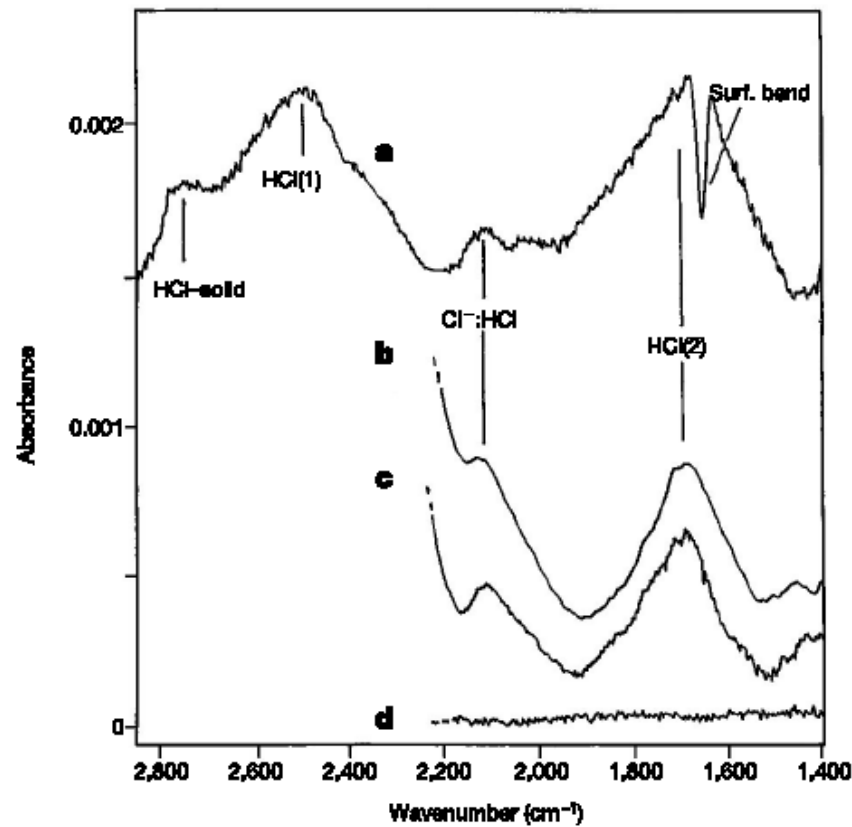
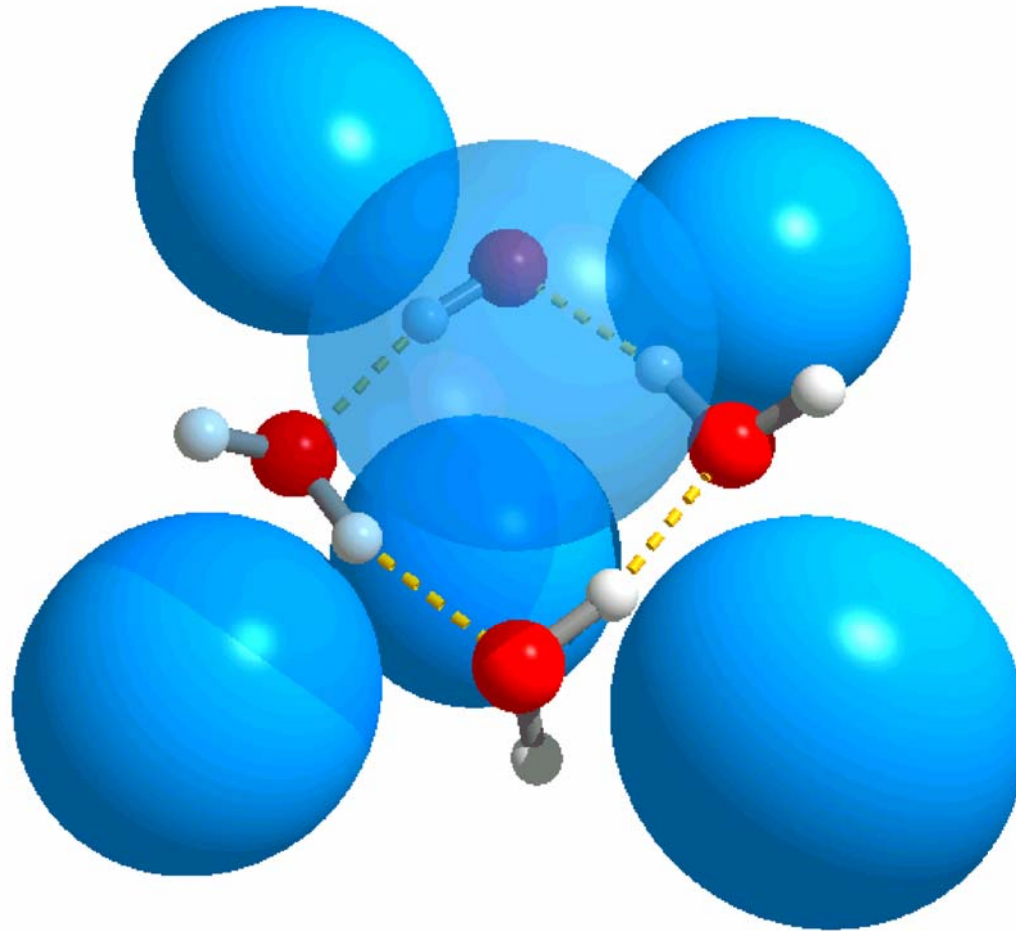
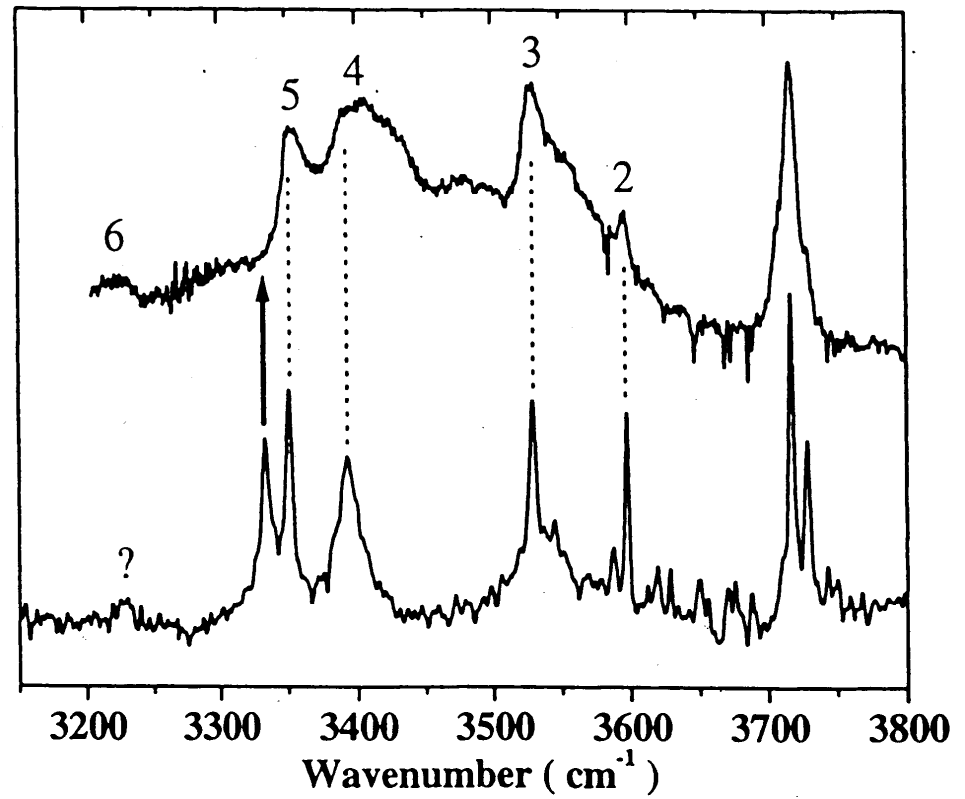
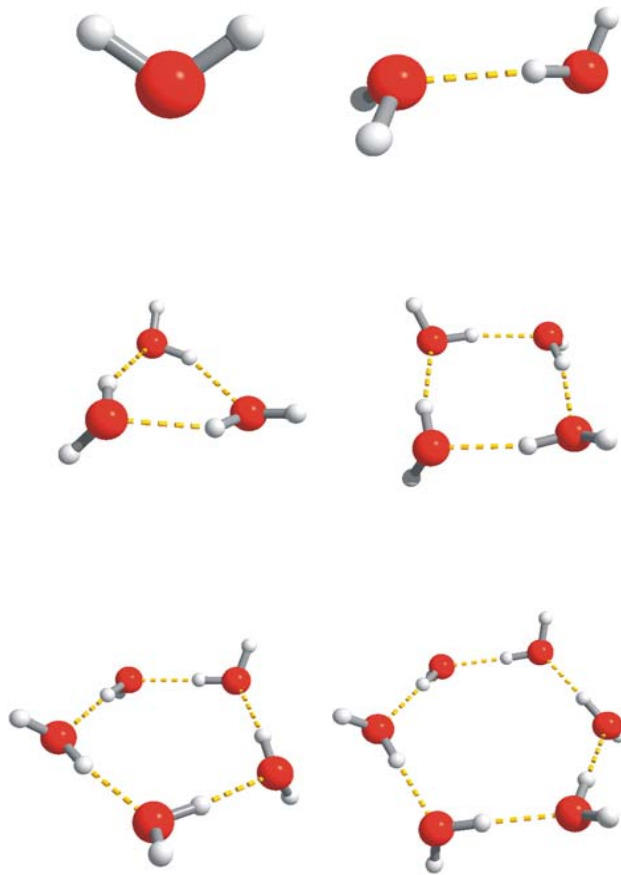


Figure 3 Cluster models used in *ab initio* calculations. The configurations and the normal frequencies were obtained on the second-order Moller–Plesset perturbation theory level in the augmented correlation consistent double zeta basis²⁷, using the Gaussian 98 program²⁸. H is shown white, Cl green, O in H₂O red, and O in H₃O⁺ yellow. Hydrogen bonds are indicated by dashed lines; those marked by arrows impede HCl solvation. The H...Cl bond lengths (in Å) are: **a**, 1.31; **b**, 1.38; **c**, 1.80; **d**, 1.84 and 1.36; **e**, 1.33; and **f**, 1.34. The HCl frequency shifts cm⁻¹ with respect to the gas phase are: **a**, -362; **b**, -1,137; **e**, -615; and **f**, -749.

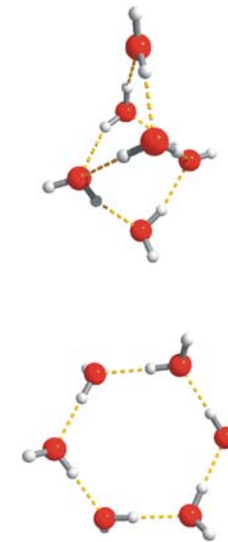
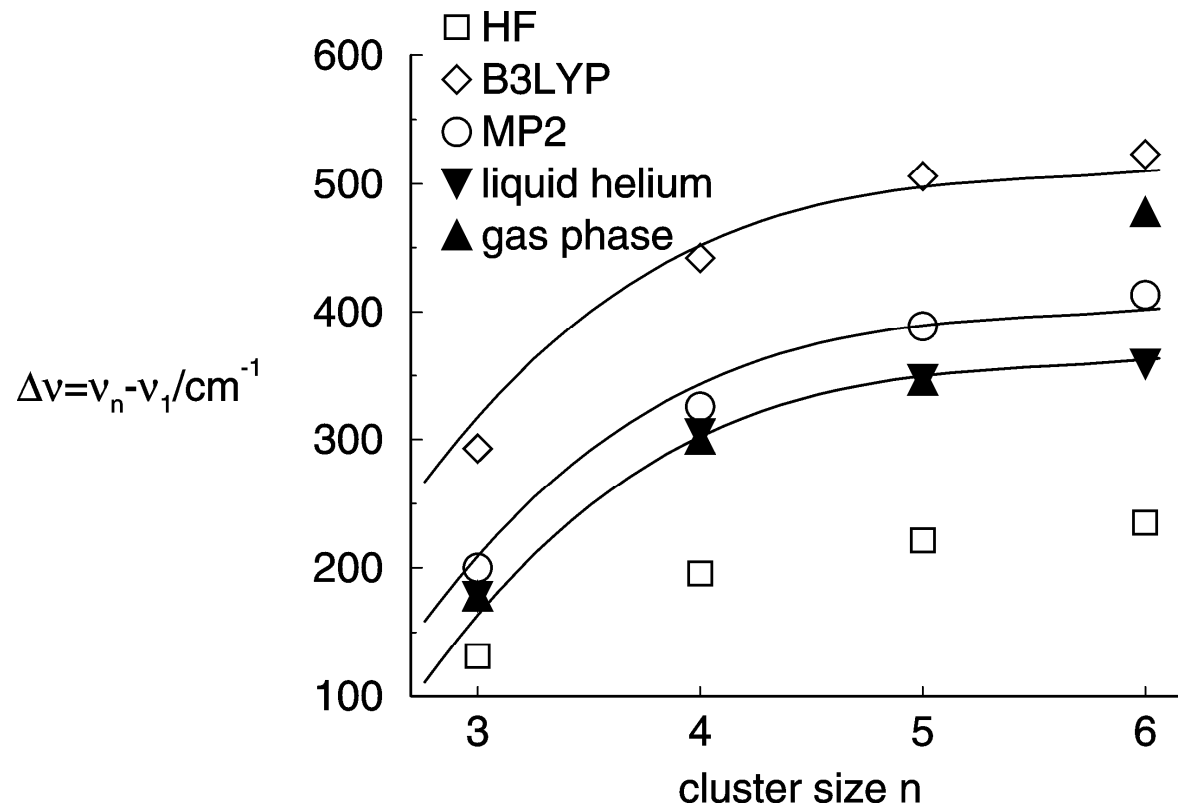
Beispiel 5: Wassercluster



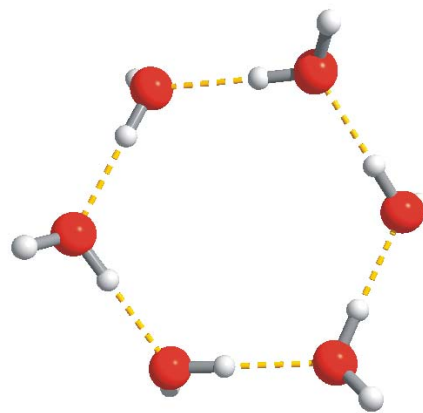
Beispiel 5: Wassercluster



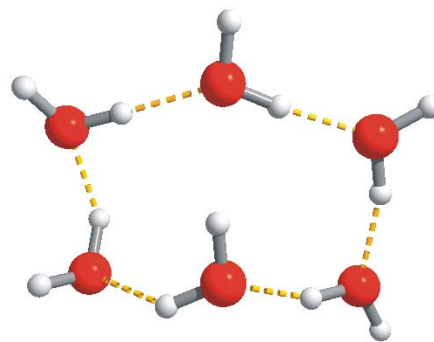
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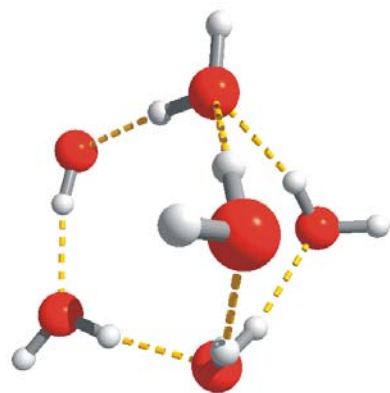
Beispiel 5: Wassercluster



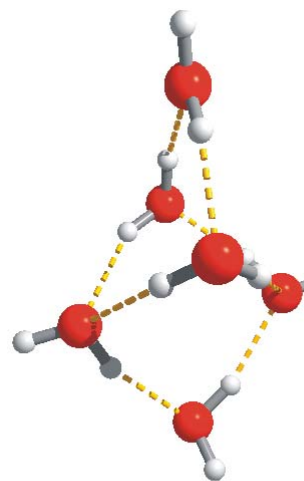
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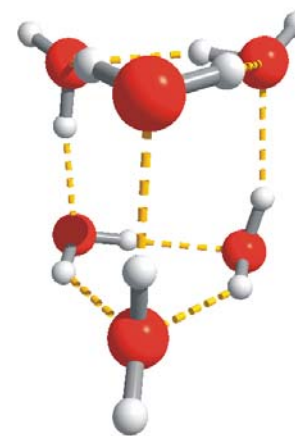
book



bag

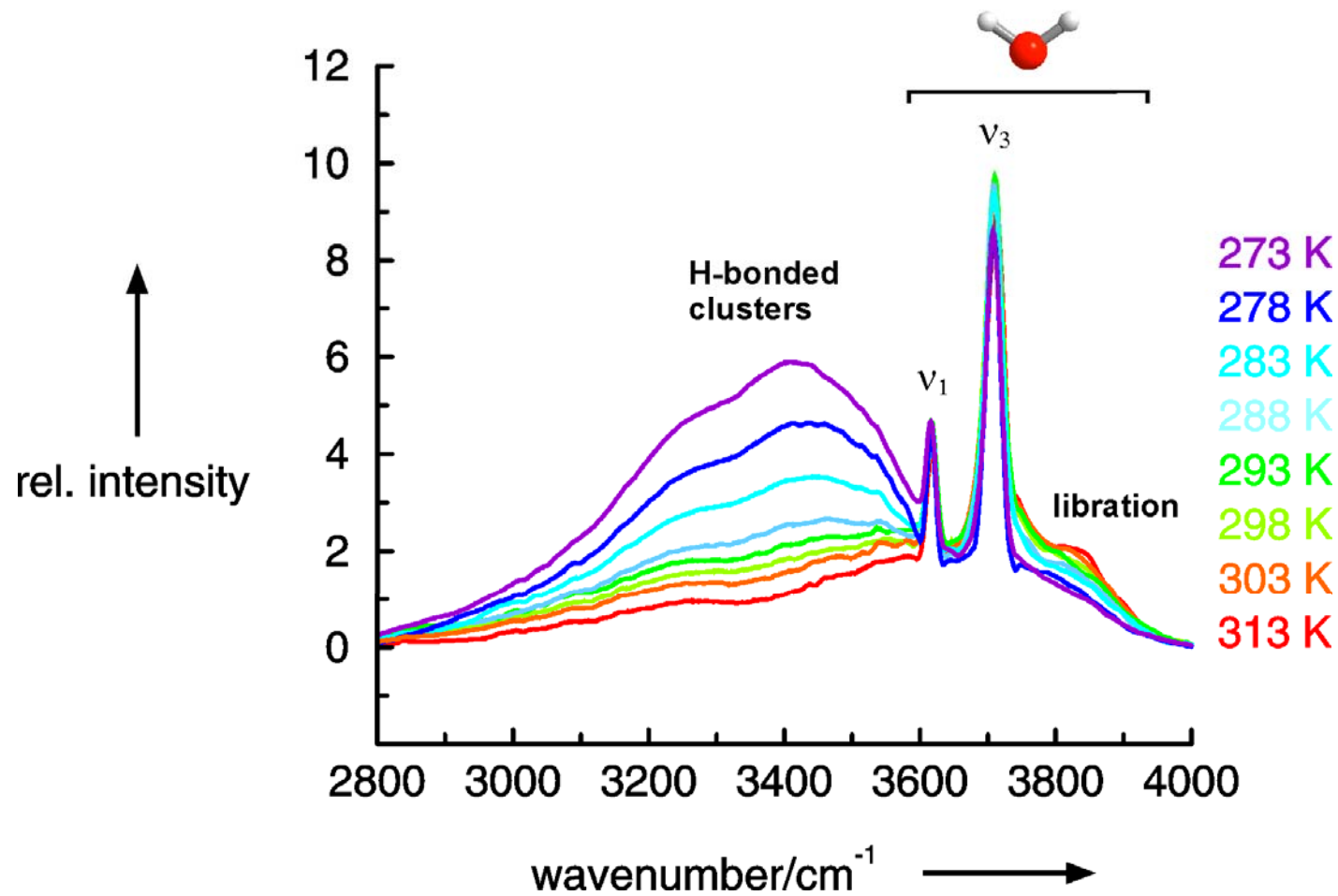


cage

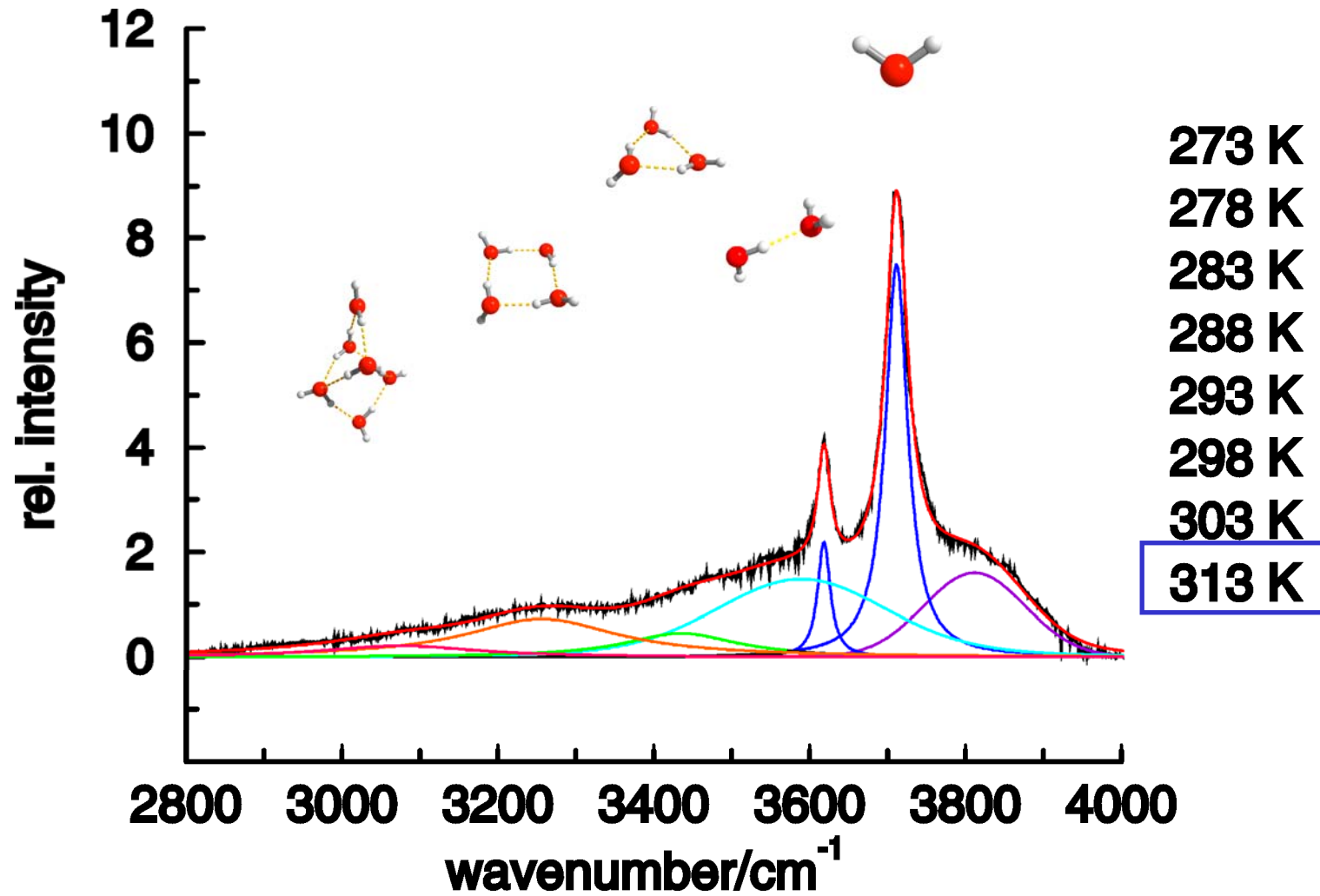


prism

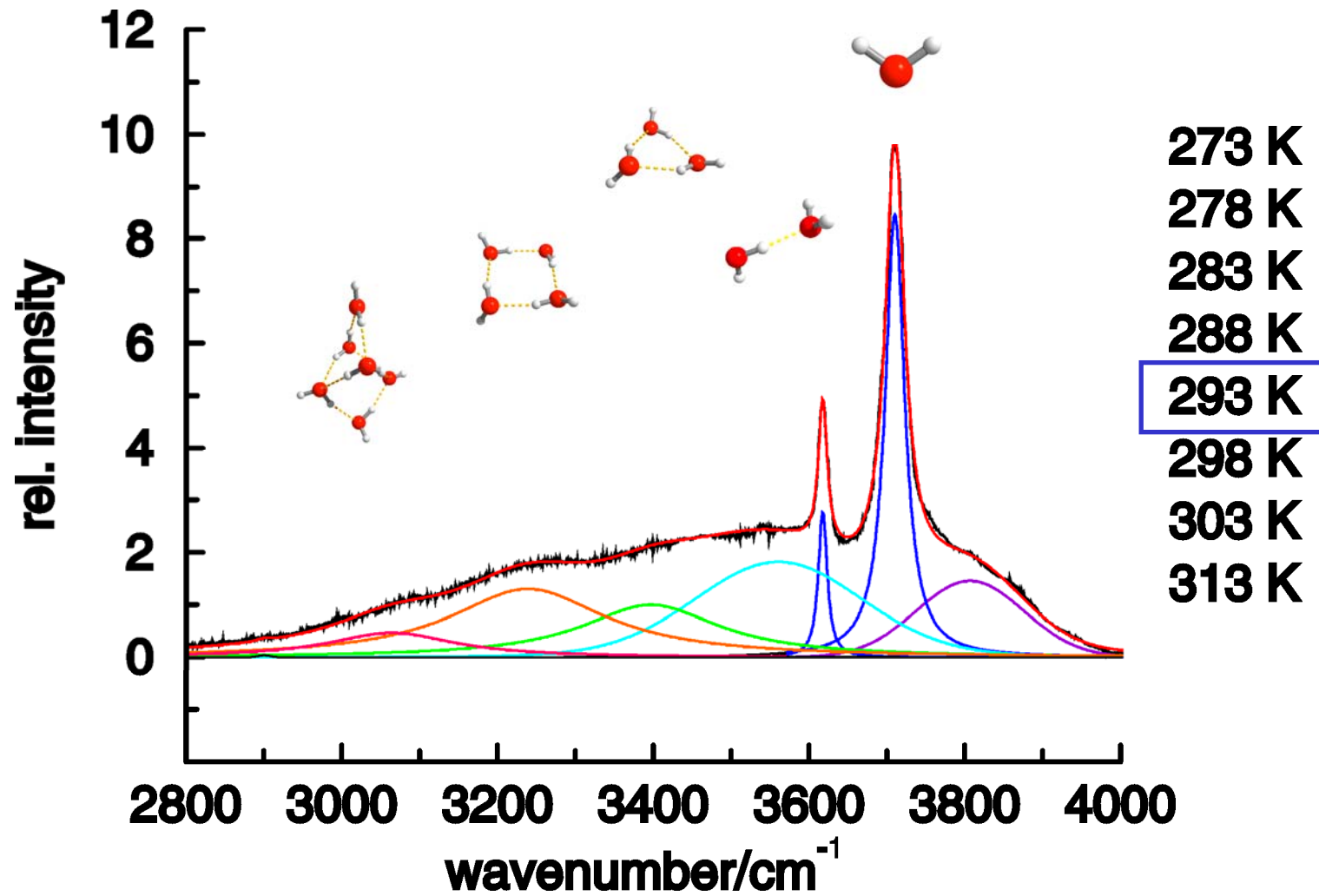
Beispiel 5: Wassercluster



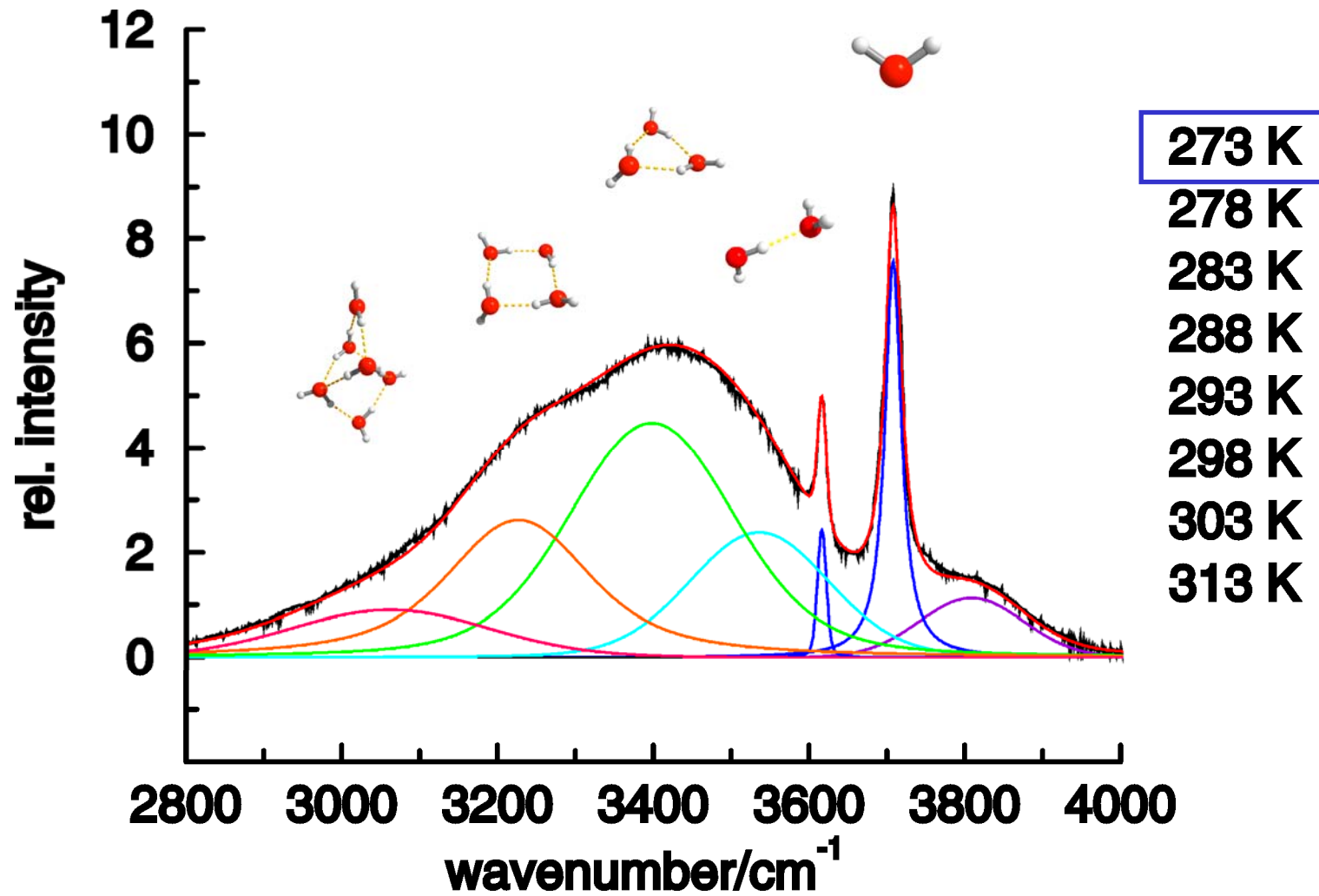
Beispiel 5: Wassercluster



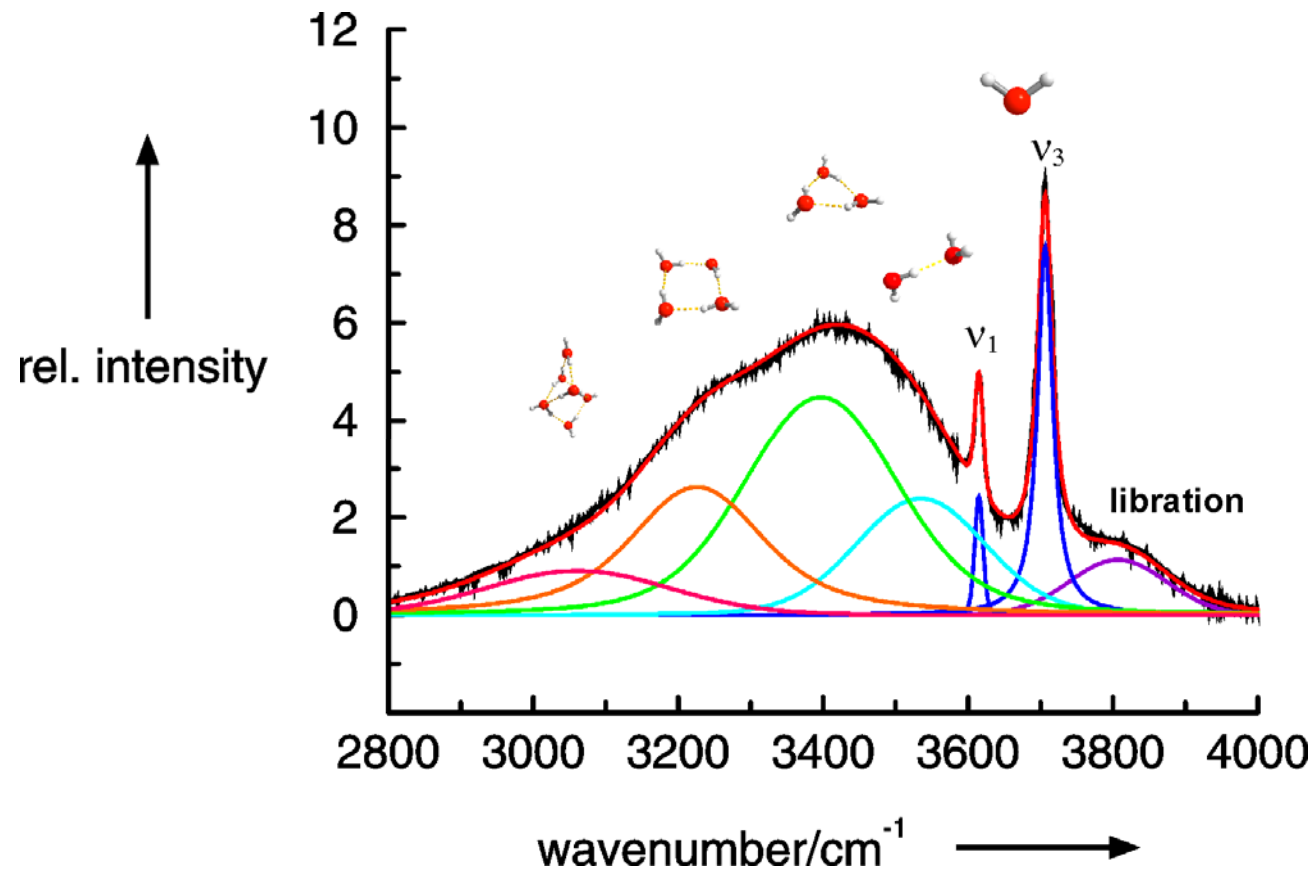
Beispiel 5: Wassercluster



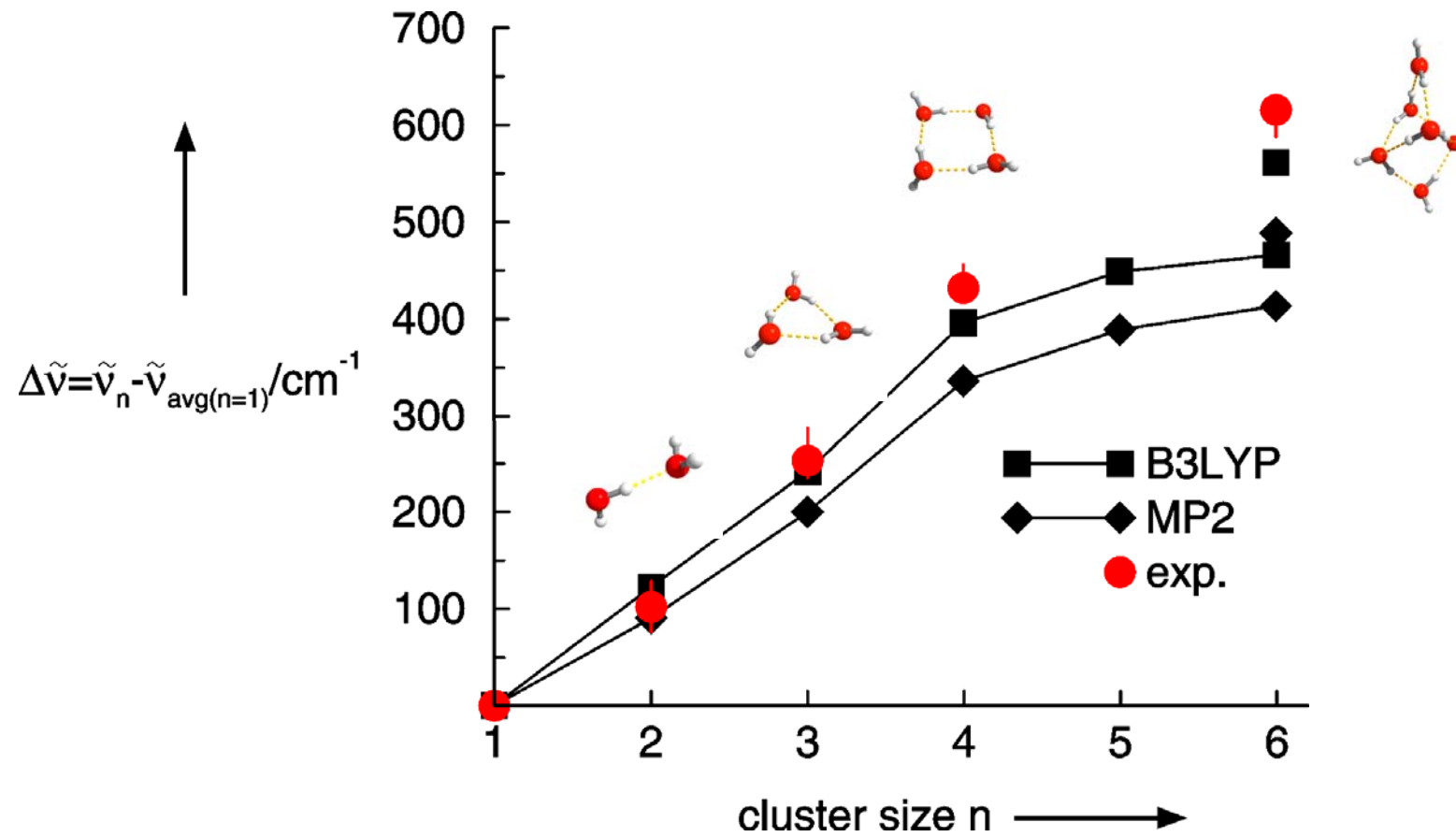
Beispiel 5: Wassercluster



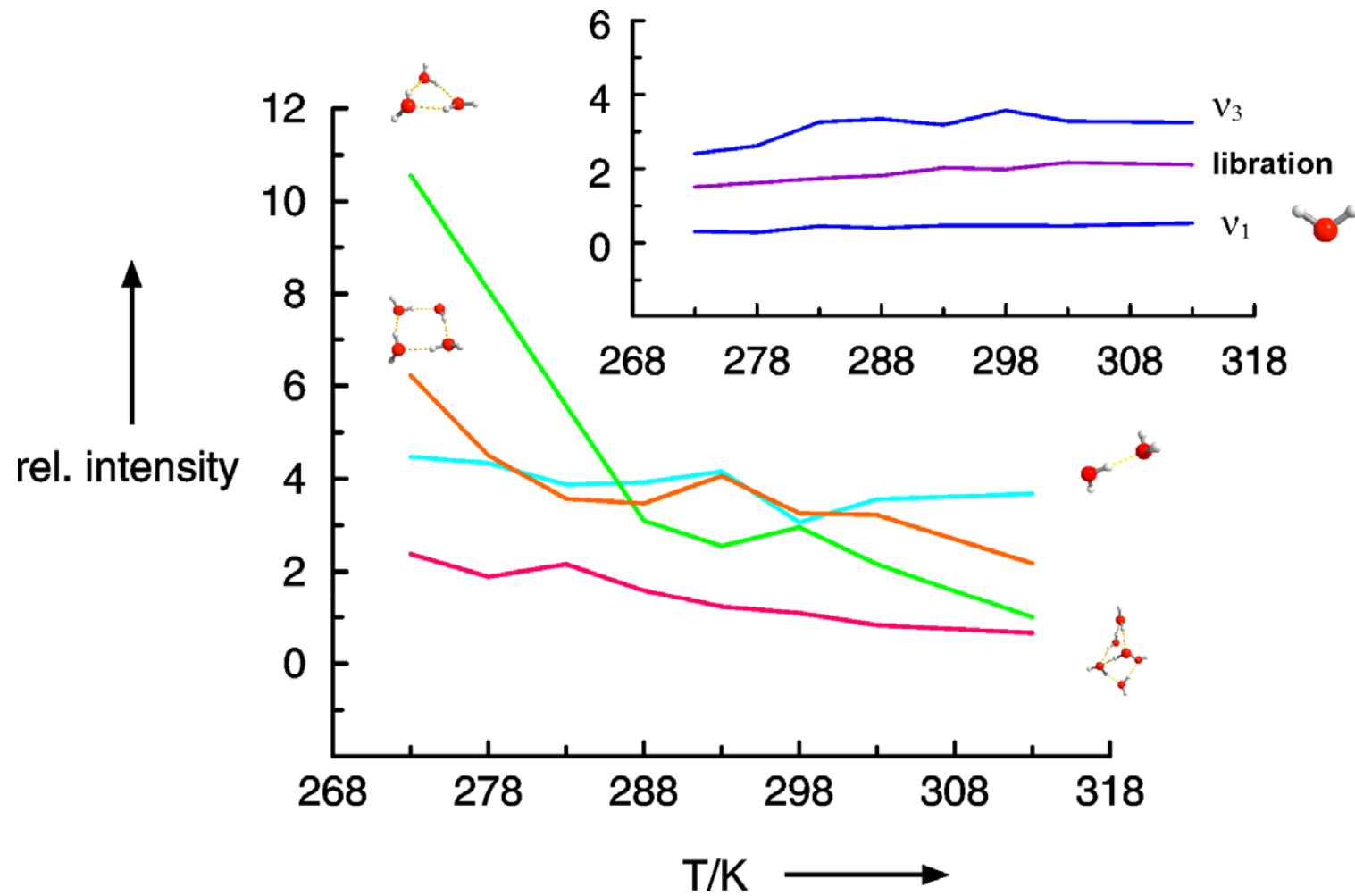
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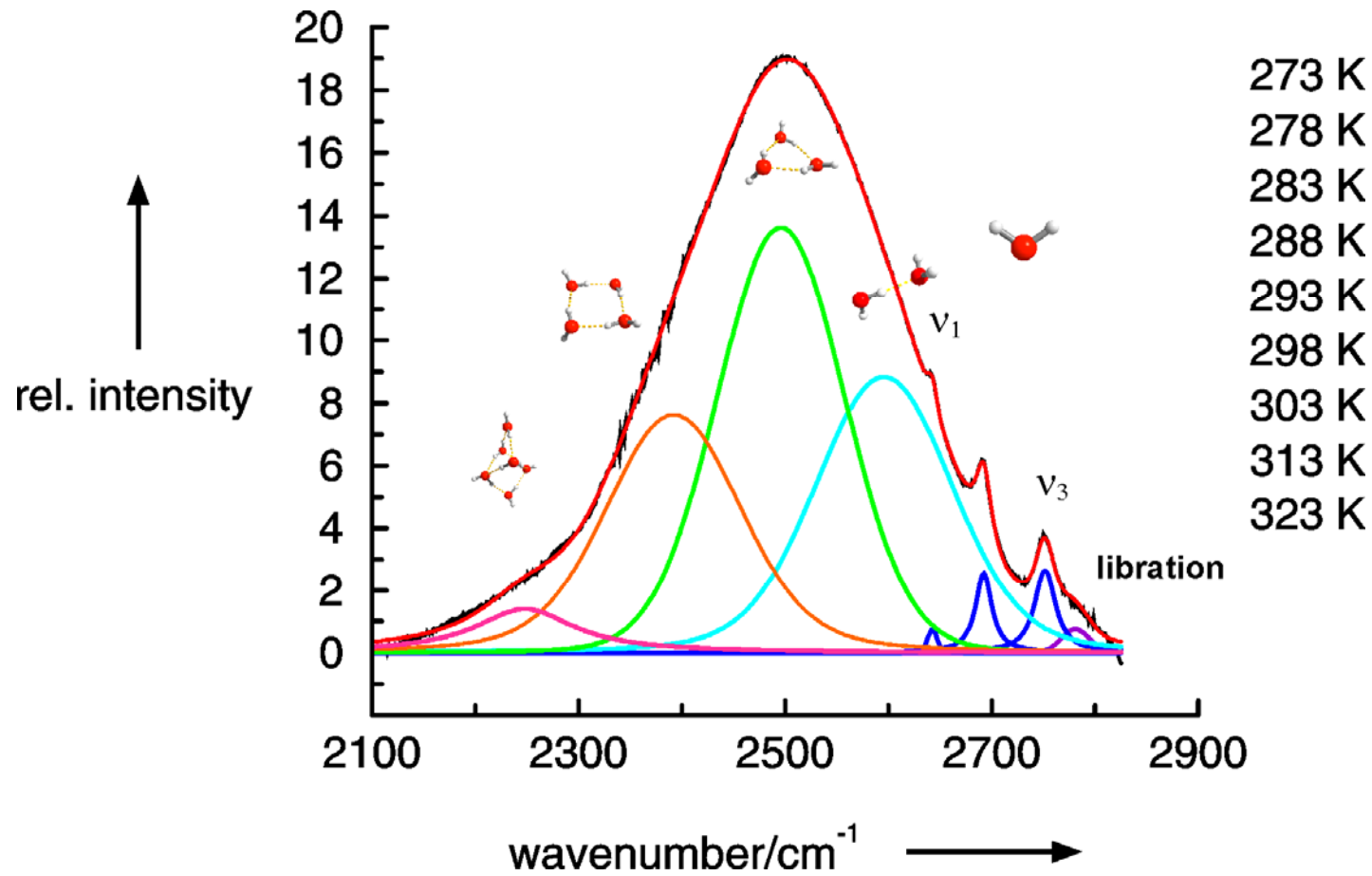
Beispiel 5: Wassercluster



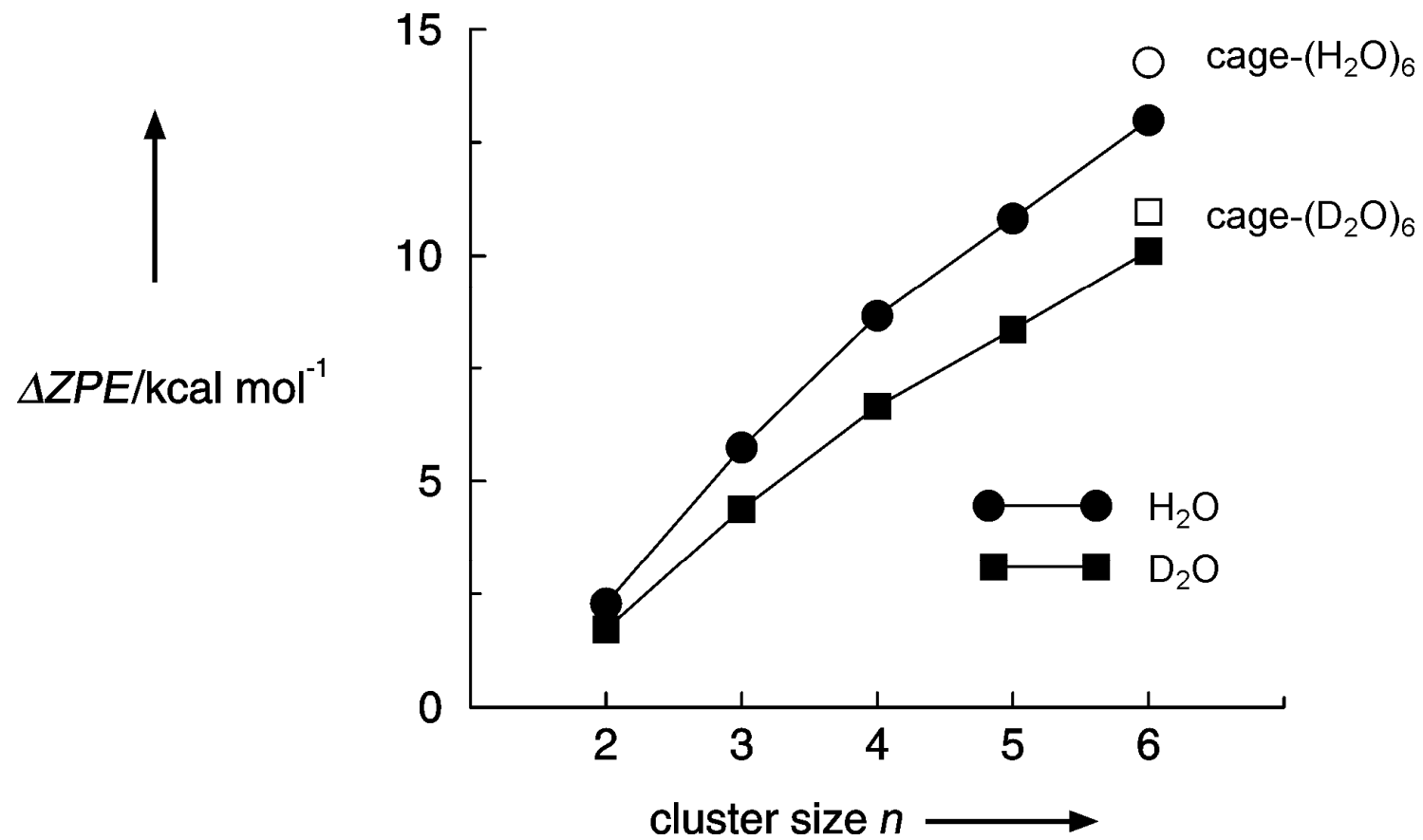
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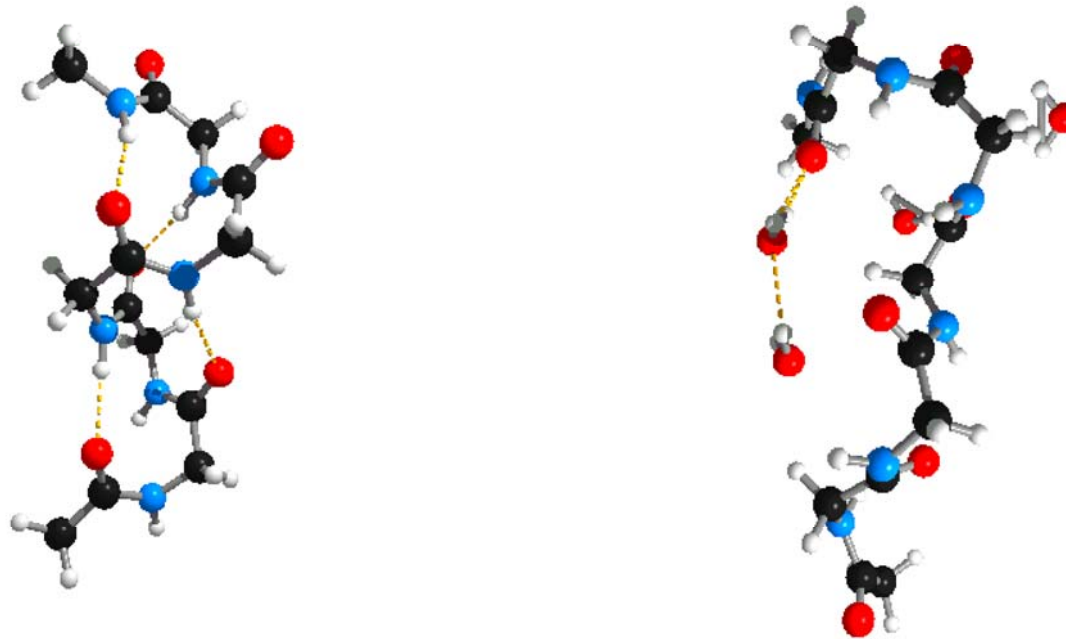
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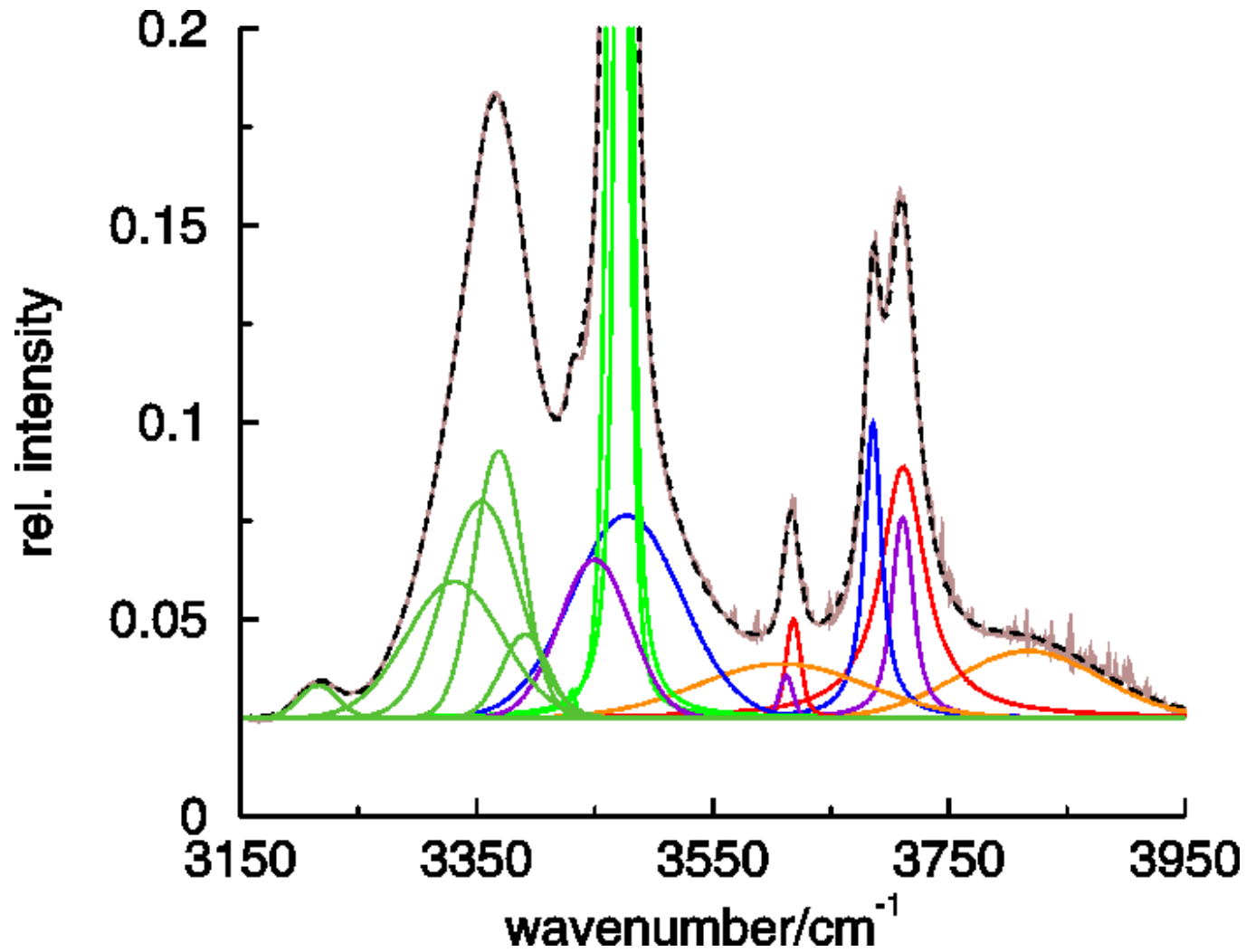
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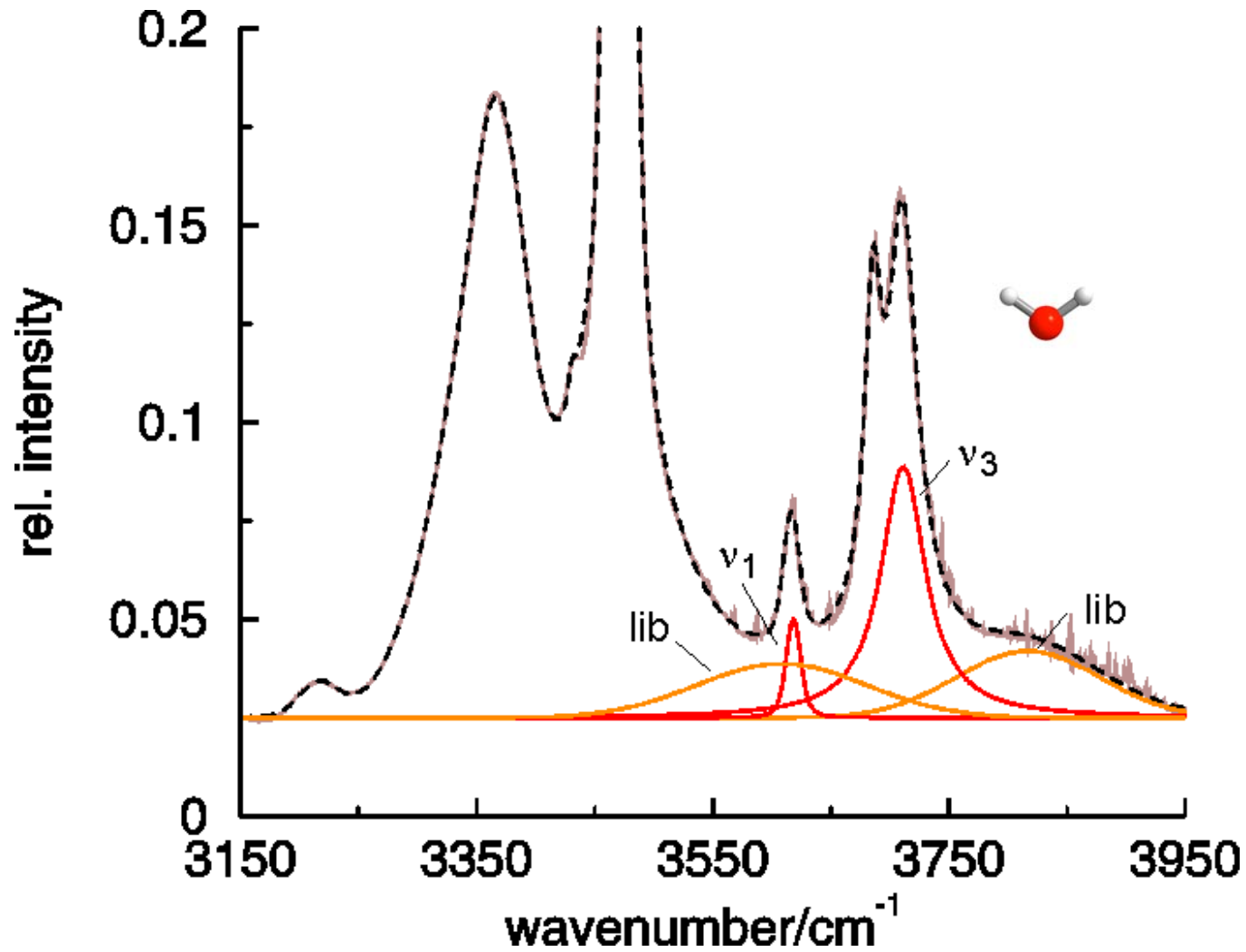
Beispiel 6: Peptid-Wasser-Wechselwirkung



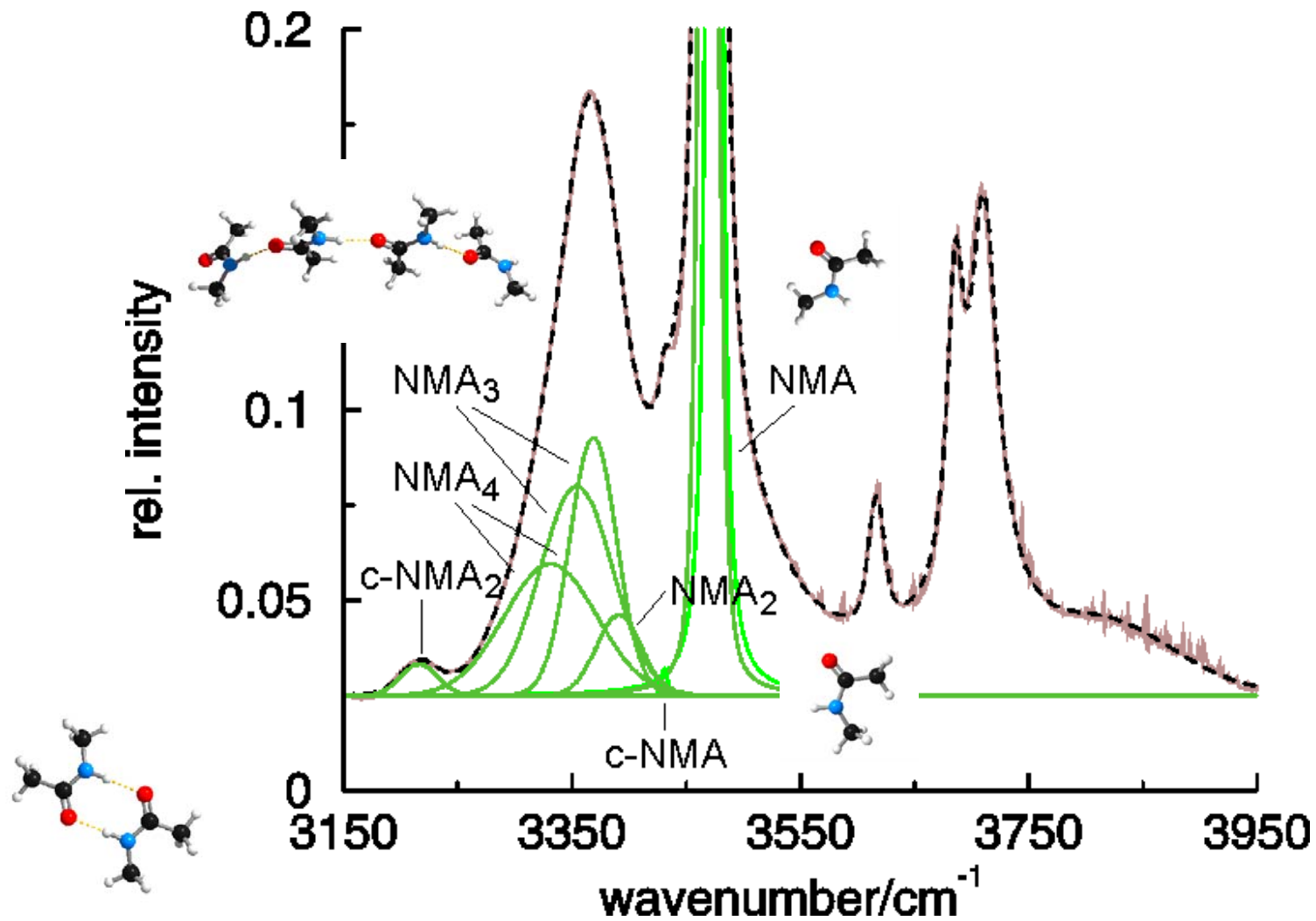
Beispiel 6: NMA-Wasser-Cluster



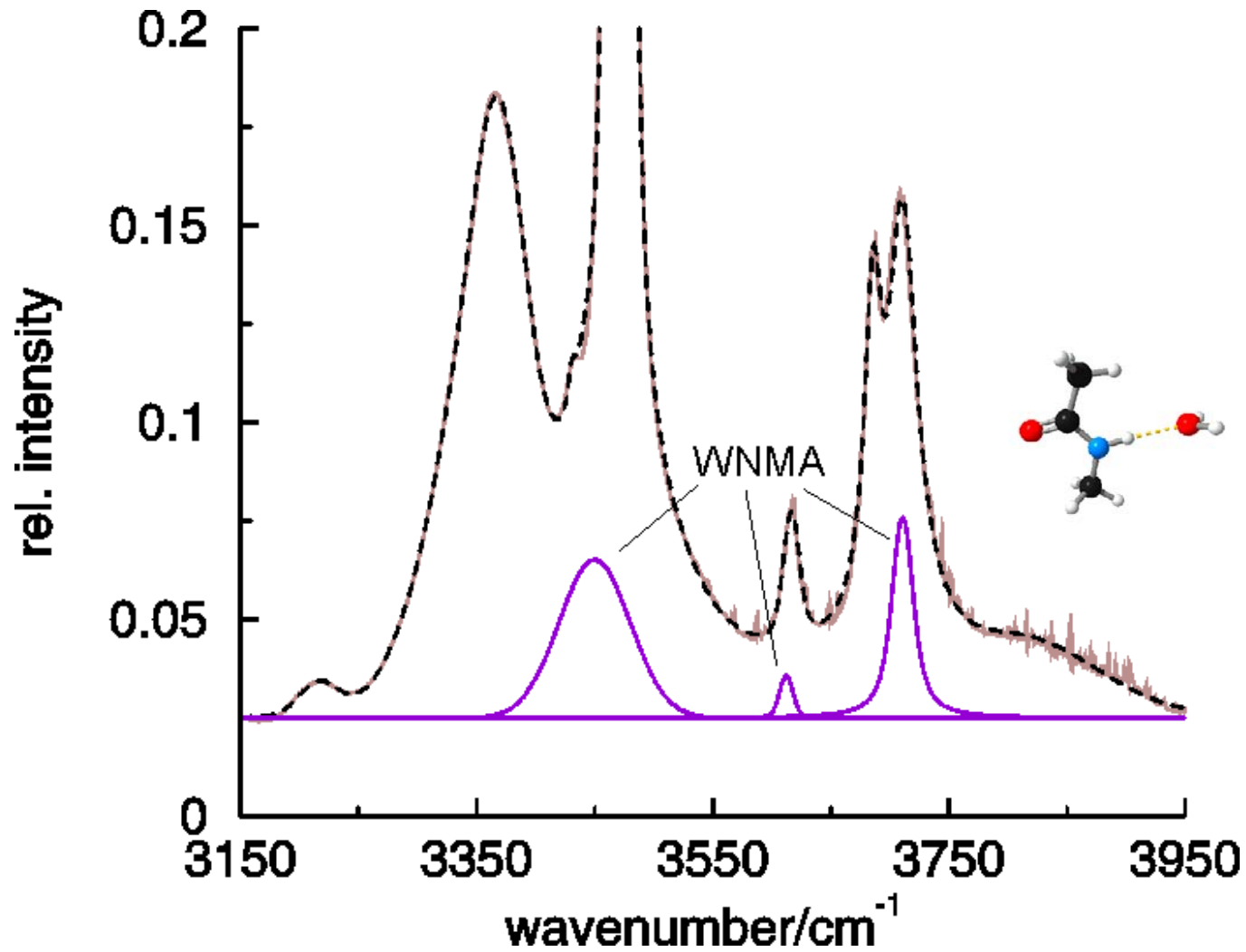
Beispiel 6: NMA-Wasser-Cluster



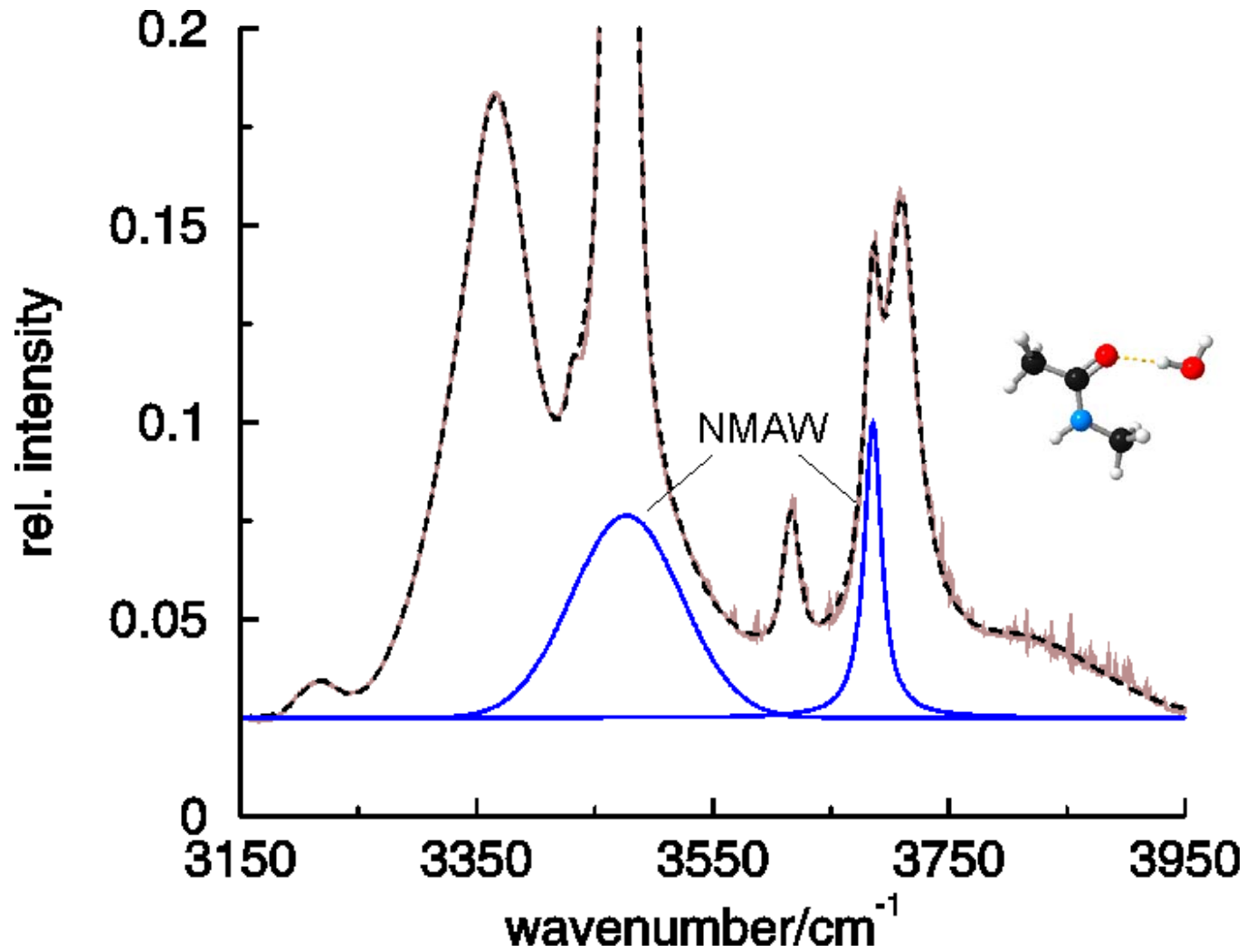
Beispiel 6: NMA-Wasser-Cluster



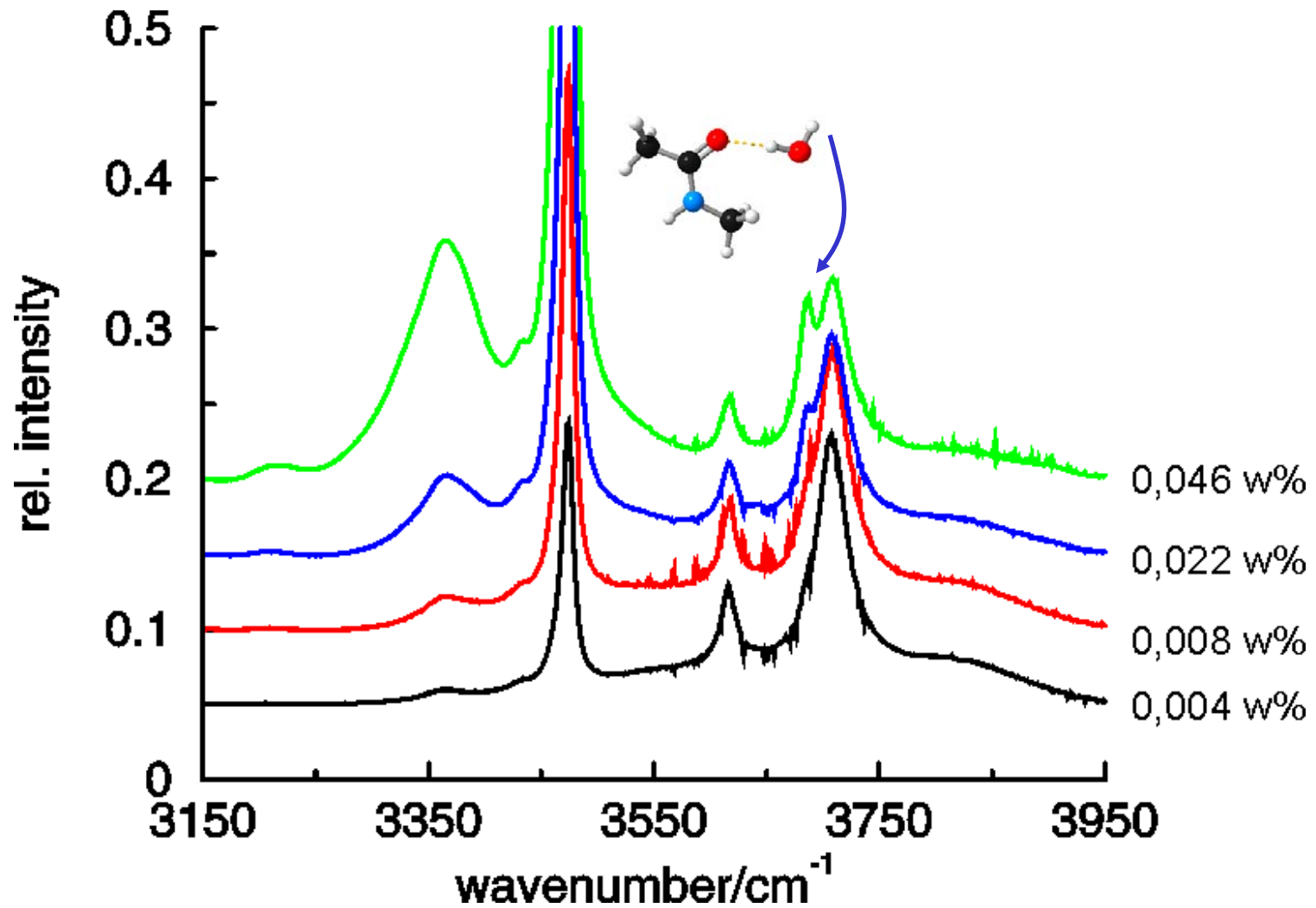
Beispiel 6: NMA-Wasser-Cluster



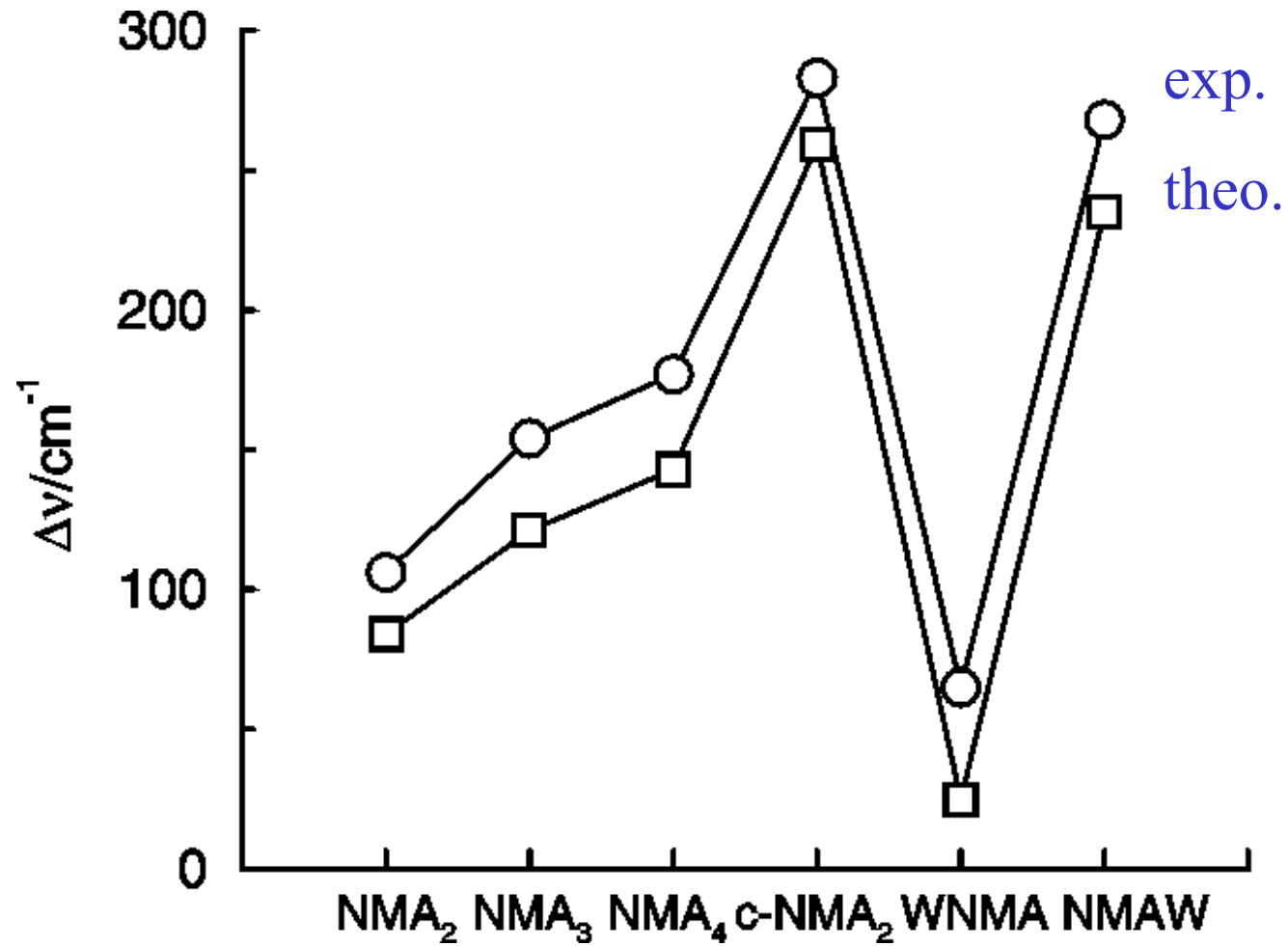
Beispiel 6: NMA-Wasser-Cluster



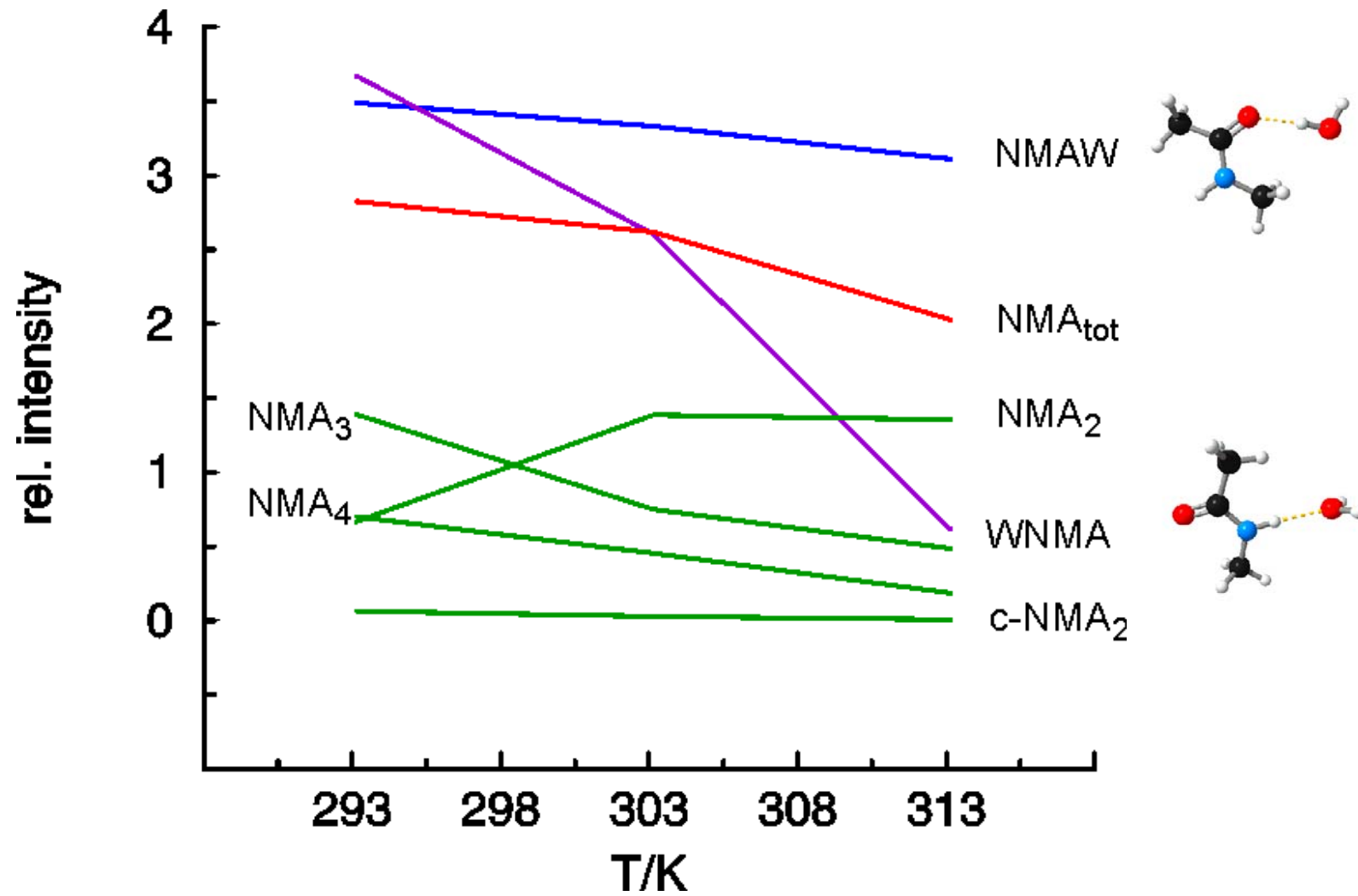
Beispiel 6: NMA-Wasser-Cluster



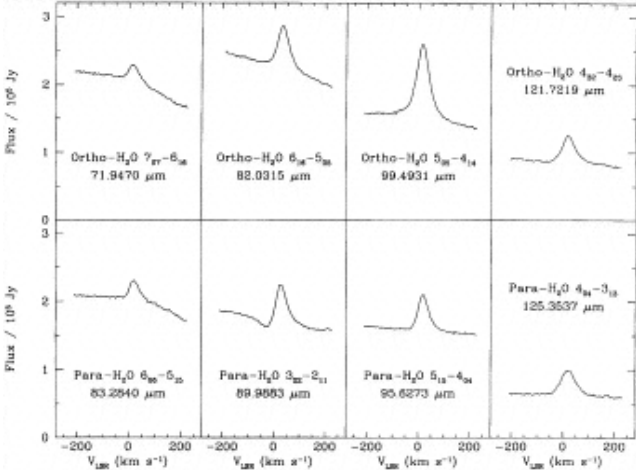
Beispiel 6: NMA-Wasser-Cluster



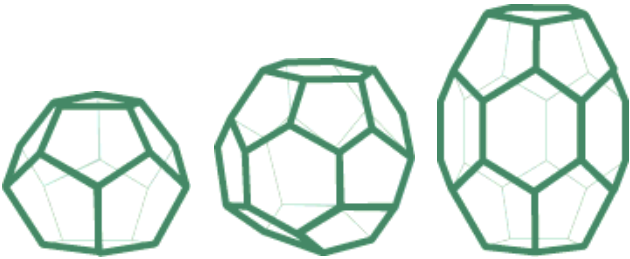
Beispiel 6: NMA-Wasser-Cluster



Beispiel 7: Weltraum

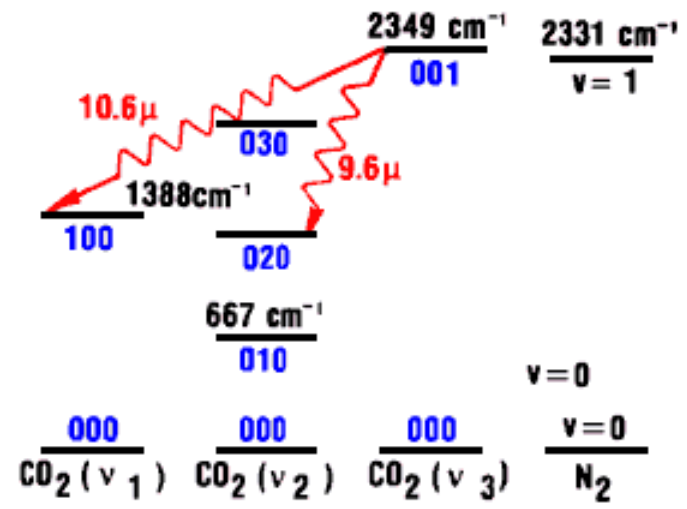
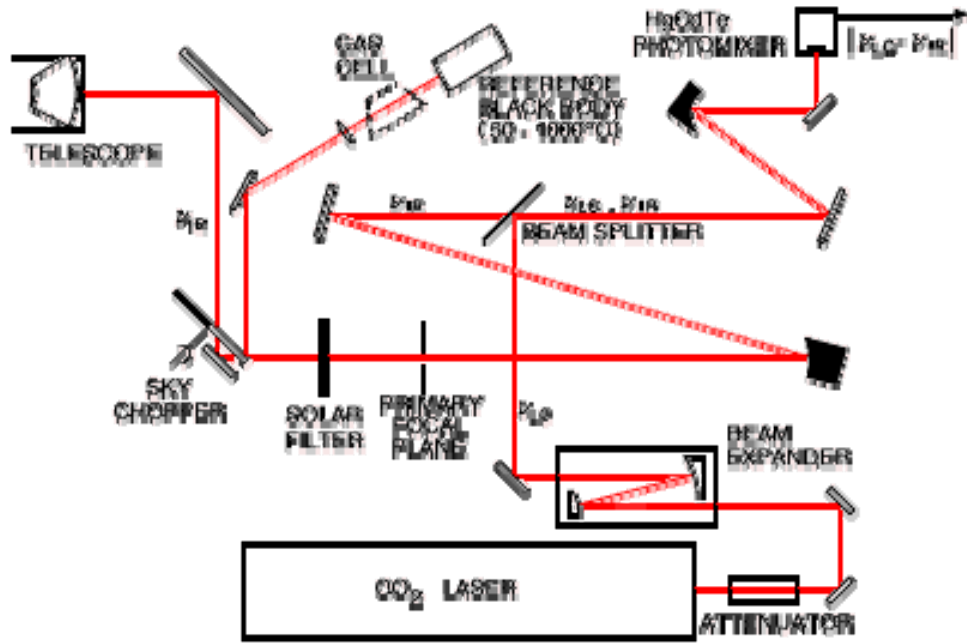


M. Harwitt, D.A. Neufeld, G.J. Melnick and M. J. Kaufman, *Astrophys. J. Lett.*, 510, 83 (1999)



"diffuse instellar bands" (DIB's) bei 35 cm⁻¹

Beispiel 7: Weltraum



Beispiel 8: Elektromagnetisches Spektrum

