Musik in bayern
ISSN: 0937-583x Volume 90, Issue 7 (July -2025)
https://musikinbayern.com DOI https://doi.org/10.15463/gfbm-mib-2025-*418*

Determination of toxic molecules (Carbon monoxide CO and Phosphine P-H) in samples of water

Mihaira H. Haddad[1]

[1]Assistant Professor, Department of Physics, Faculty of Art and Sciences in Wadi Al-Dawasir - Prince Sattam bin Abdulaziz University, Saudi Arabia
Corresponding Author Email: m.haddad@psau.edu.sa / miherahaddad@gmail.com

To Cite this Article

Mihaira H. Haddad[1],” **Determination of toxic molecules (Carbon monoxide CO and Phosphine P-H) in samples of water**” *Musik In Bayern, Vol. 90, Issue 7, July 2025, pp25-37*

Article Info
Received: 13-05-2025 Revised: 14-06-2025 Accepted: 25-06-2025 Published: 10-07-2025

Abstract:

The challenges of countries of the 21st century are to provide fresh water, water that does not contain pollutants, water that does not contain those toxic molecules that spoil its suitability.

Water contaminated with these toxic particles negatively affects human health and causes many chronic diseases such as cancer, Kidney failure and other deadly diseases, was well as negatively affects the soil and livestock.

I chose a number of areas in northern Sudan as a study area because these areas have a large number of factories, as well as area where gold is mined and extracted with mercury and cyanide. Also, northern Sudan is an agricultural area and farmers there use many pesticides and chemical fertilizers.

All the above-mentioned industrial, agricultural or mining activities increase the possibility of water being contaminated with some toxic molecules.

The following parameters were tested:

(Carbon monoxide CO, Phosphine P-H and Nitrate NO).

The results showed the presence of these molecules in the studied samples.

Musik in bayern
ISSN: 0937-583x Volume 90, Issue 7 (July -2025)
https://musikinbayern.com DOI https://doi.org/10.15463/gfbm-mib-2025-*418*
Keywords: Raman Spectroscopy, Water contamination, Carbon monoxide, Phosphine and Nitrate.

Declaration of Interest Statement:

The authors extend their appreciation to the deputyship for research & innovation, ministry of education in Saudi Arabia for funding this research work through the project number (IF2/PSAU/ 2022/01/23000)"

1. introduction

Water with the chemical formula H_2O is a polar inorganic compound. It is a tasteless and odorless liquid at room temperature and is the basis of the fluids of living organisms. It is classified as the most studied chemical compound and is described as the "universal solvent" for its ability to dissolve many substances. [1]

Water is considered polluted when it is mixed with some toxic molecules or elements, which reduces the quality of the water and makes it unfit for use.

To study quality of water whether it contaminated or fit for use, we need very precise techniques that have ability to identifying the components of the substance under study and detecting the contaminants present in it.

2. Stimulated Absorption of Radiation

When an electromagnetic radiation falls on matter (typically electrons bound in atoms) takes up a photon's energy and so transforms electromagnetic energy into internal energy of the absorber. [2]

This suggests that specific frequencies of incident energy are absorbed by the atoms.

$$dN_1 = -B_{12}\rho(v_o)N_1 dt \qquad (1)$$

Where $\rho(v_0)$ is the range energy thickness of radiation at frequencies close (v_0), $N_1$is the number of inhabitants in the ground state, N_2 is the number of

Musik in bayern
ISSN: 0937-583x Volume 90, Issue 7 (July -2025)
https://musikinbayern.com DOI https://doi.org/10.15463/gfbm-mib-2025-*418*

inhabitants in molecules in the energized state, and B_{12} is the Einstein coefficient of retention. Just within the sight of a field is retention possible; the course of ingestion is upgraded.

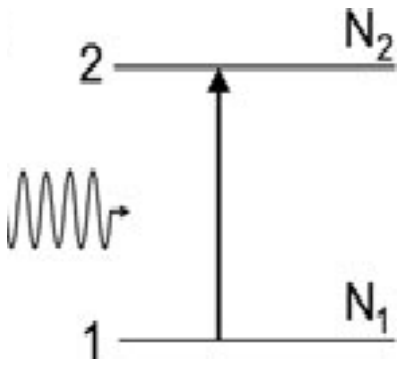


Figure (1) Stimulated Absorption

3. Emission of Radiation

3.1. Spontaneous Emission of Radiation

Spontaneous emission is the process in a molecule, an atom or a subatomic particle transits from an excited energy state E_2 to a lower energy state E_1 (e.g., its ground state) and emits a quantized amount of energy in the form of a photon. [3]

The well-known expression then yields the frequency of the emitted wave,(v_0) :

$$v_0 = \frac{E_2 - E_1}{h} \qquad (2)$$

where h is Planck's constant.

$$dN_2 = -A_{21} N_2 dt \qquad (3)$$

Musik in bayern
ISSN: 0937-583x Volume 90, Issue 7 (July -2025)
https://musikinbayern.com DOI https://doi.org/10.15463/gfbm-mib-2025-*418*

Where A_{21} is the spontaneous emission Einstein coefficient. The upper level's population declines exponentially

$$N_2 = N_2(0)e^{-A_{21}t} = N_2(0)e^{-t/\tau_{sp}} \qquad (4)$$

N_2 (0) is the thickness of excited two-level nuclear frameworks at time zero, and is the usual lifespan of an energetic two-level atomic framework regarding unrestrained discharge (=spontaneous lifetime sp). We have the straightforward relation

$$A_{21} = 1/\tau_{sp} \qquad (5)$$

The reciprocal of the spontaneous lifespan is the Einstein coefficient A_{12}.

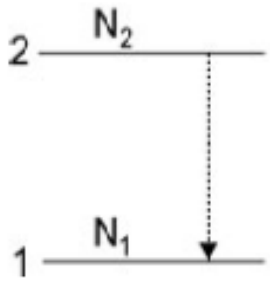


Figure (2): Spontaneous emission

3.2. Stimulated Emission of Radiation

Stimulated emission is the process by which an incident photon of a certain frequency can interact with an excited atomic electron in E_2 level causing it to drop to a lower energy level E_1. The released energy is transmitted into the electromagnetic field, creating a new photon that has frequency, polarization, and direction, all of which are identical to the photons of the incident wave. [4]

$$dN_2 = -B_{21}\rho(v_o)N_2dt \qquad (6)$$

Musik in bayern
ISSN: 0937-583x Volume 90, Issue 7 (July -2025)
https://musikinbayern.com DOI https://doi.org/10.15463/gfbm-mib-2025-*418*

Where B_{21} is the stimulated emission Einstein coefficient. As per figure, the radiation delivered by invigorated outflow has a similar recurrence, polarization, course, and stage as the invigorating radiation (1.3).

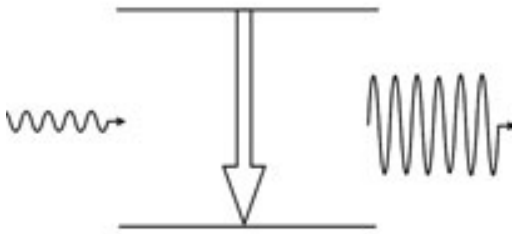


Figure (3) Stimulated Emission

4. Spectroscopy

Is the science of studying the interaction between Electromagnetic Radiation (energy) and matter is called spectroscopy which can be used to obtain information about the identity and structure of substances. It is generally involve measurements of two experimental parameters: The energy of the radiation absorbed or emitted by the system and the Intensity of the spectral lines. [5]

Spectroscopy is mainly used for studying the structure of molecules and atoms. It will use a large wavelength to investigate the structure and electron configurations of atoms and molecules.

Spectroscopy can also be used for finding the unknown chemical composition of materials. Spectroscopy's emission spectrum will help to concentrate on a few parts per million of a trace element in a material.

Spectroscopy also can be classified into two types by the nature of the interaction between the energy and the matter. These interactions include: [6]

Absorption spectroscopy: Absorption occurs when energy from the radiative source is absorbed by the material. Absorption is often determined by measuring the fraction of energy transmitted through the material, with absorption decreasing the transmitted portion.

Emission spectroscopy: Emission indicates that radiative energy is released by the material. A material's blackbody spectrum is a spontaneous emission spectrum determined by its temperature. This feature can be measured in the infrared by instruments such as the atmospheric emitted radiance interferometer.[18] Emission can also be induced by other sources of energy such as flames, sparks, electric arcs or electromagnetic radiation in the case of fluorescence. [7]

There are different types of spectroscopic techniques such as:

IR Spectroscopy, UV Spectroscopy, Mass Spectroscopy, Fluorescence Spectroscopy, FTIR Spectroscopy, Laser Induced Spectroscopy and Raman Spectroscopy.

5. Raman Spectroscopy

Raman spectroscopy is a scattering technique. It is involves the study of transitions between quantum levels of molecules and matter induced by the inelastic scattering of light. [8]

In Raman spectroscopy, sample is illuminated with a monochromatic laser beam which interacts with the molecules of sample and originates a scattered light. The scattered light having a frequency different from that of incident light ***(inelastic scattering)*** is used to construct a Raman spectrum. Raman spectra arise due to inelastic collision between incident monochromatic radiation and molecules of sample. When a monochromatic radiation strikes at sample, it scatters in all

ISSN: 0937-583x Volume 90, Issue 7 (July -2025)
https://musikinbayern.com **DOI https://doi.org/10.15463/gfbm-mib-2025-*418***

directions after its interaction with sample molecules. Much of this scattered radiation has a frequency which is equal to frequency of incident radiation and constitutes ***Rayleigh scattering***. Only a small fraction of scattered radiation has a frequency different from frequency of incident radiation and constitutes ***Raman scattering.*** When the frequency of incident radiation is higher than frequency of scattered radiation, ***Stokes lines*** appear in Raman spectrum. But when the frequency of incident radiation is lower than frequency of scattered radiation, ***anti-Stokes lines*** appear in Raman spectrum. Scattered radiation is usually measured at right angle to incident radiation. [9, 10]

Stokes shifted Raman bands involve the transitions from lower to higher energy vibrational levels and therefore, Stokes bands are more intense than anti-Stokes bands and hence are measured in conventional Raman spectroscopy while anti-Stokes bands are measured with fluorescing samples because fluorescence causes interference with Stokes bands. The magnitude of Raman shifts does not depend on wavelength of incident radiation.[3] Raman scattering depends on wavelength of incident radiation. A change in polarizability during molecular vibration is an essential requirement to obtain Raman spectrum of sample. Since Raman scattering due to water is low, water is an ideal solvent for dissolving samples. Glass can be used for optical components (mirror, lens, sample cell) in Raman spectrophotometer. [9, 10]

Musik in bayern
ISSN: 0937-583x Volume 90, Issue 7 (July -2025)
https://musikinbayern.com DOI https://doi.org/10.15463/gfbm-mib-2025-*418*

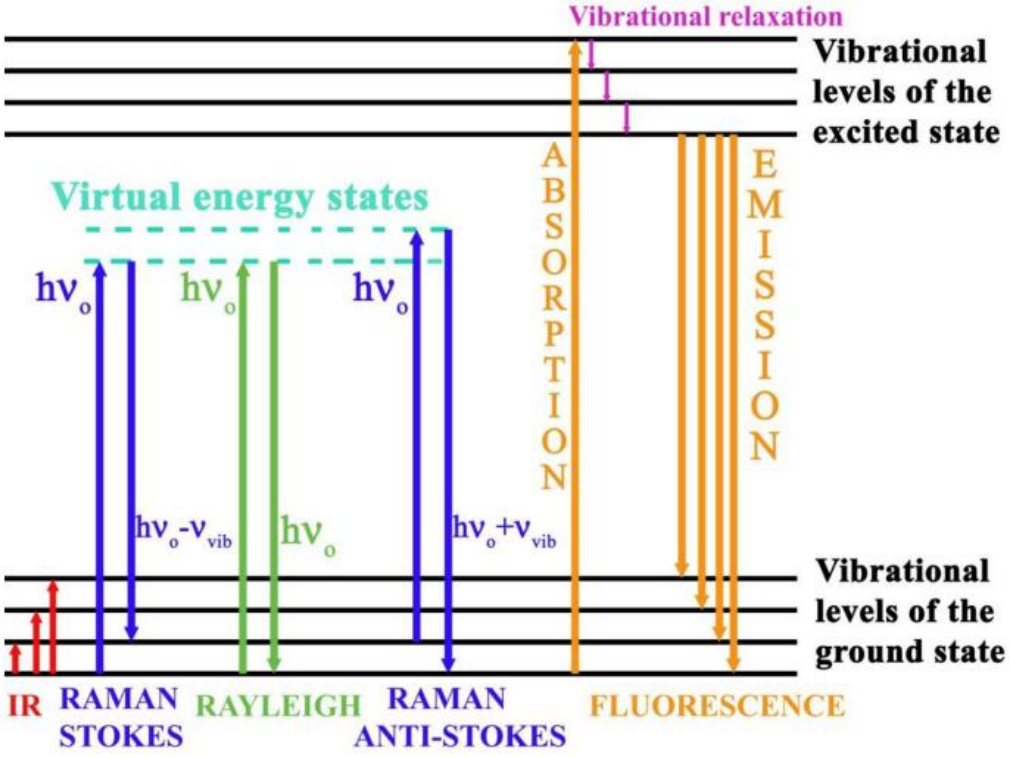


Figure (4) Vibrational and electronic energy-level diagram of a molecule showing the processes of IR absorption, Raman and Rayleigh scattering and fluorescence emission.

6. Material and method

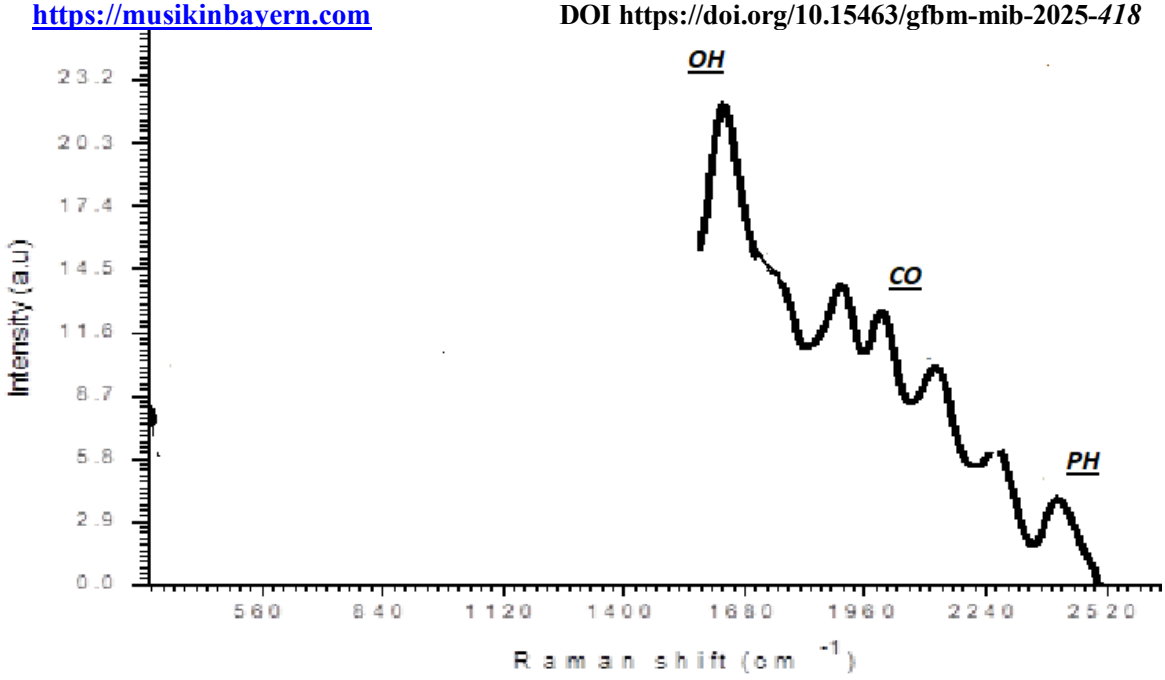
   Three water samples were collected from three different regions in Sudan for the purpose of detecting contaminants present in them.

The samples were studied using a Raman spectrometer, and the Raman spectra resulting from the reaction were recorded, and the contaminated molecules were identified by referring to the references.

7. Results

According to the findings, these samples also include other hazardous chemicals in varying levels in addition to the water.

Musik in bayern
ISSN: 0937-583x Volume 90, Issue 7 (July -2025)
https://musikinbayern.com DOI https://doi.org/10.15463/gfbm-mib-2025-*418*

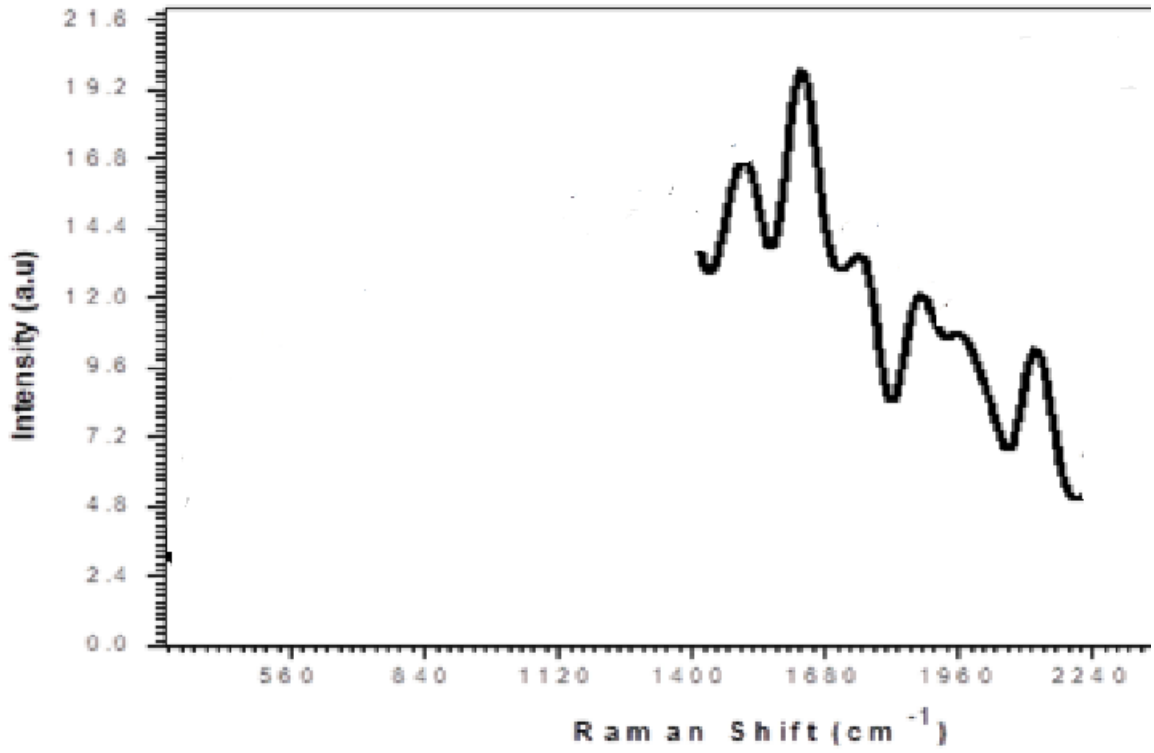


Finger (5) Raman spectra of sample 1

Table 1 molecules in sample 1

Wavenumber **(cm^{-1})**	**Intensity (a.u)**	Type of molecules
1635	22.19	OH bending
1899.4	13.94	C O
2403	4.02	PH

Musik in bayern
ISSN: 0937-583x Volume 90, Issue 7 (July -2025)
https://musikinbayern.com DOI https://doi.org/10.15463/gfbm-mib-2025-*418*

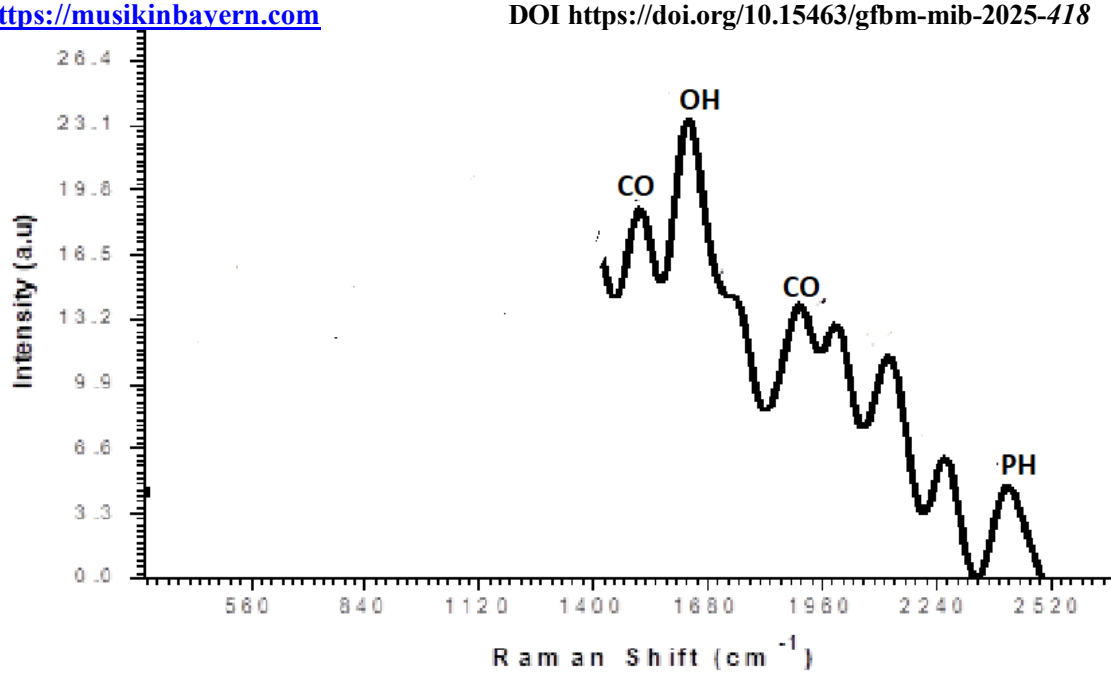


Finger (6) Raman spectra of sample 2

Table 2 molecules in sample 2

Wavenumber **(cm^{-1})**	**Intensity (a.u)**	Type of molecules
1510.9	16.84	CO
1635	19.97	OH bending

Musik in bayern
ISSN: 0937-583x Volume 90, Issue 7 (July -2025)
https://musikinbayern.com DOI https://doi.org/10.15463/gfbm-mib-2025-*418*



Finger (7) Raman spectra of sample 1

Table 3 molecules in sample 3

Wavenumber **(cm^{-1})**	**Intensity (a.u)**	Type of molecules
1510.9	18.93	CO
1635	23.56	OH bending
1899.4	14.02	CO
2411.6	4.79	PH

8. Discussion

After the study, it was found that the studied water samples contain pollutants **(Carbon monoxide CO and Phosphine P-H** molecules**)**, as shown in the figures below.

These pollutants appeared in significant quantities, as shown in the tables below. The peak at 1635 cm^{-1} appeared in the three spectra, indicating that the sample

studied was water.

9. Recommendations

The competent government agencies must raise the quality of water by increasing the number of water purification plants.

As well as holding workshops and lectures to explain to citizens in those areas the danger of using polluted water.

10. References

1. Greenwood NN, Earnshaw A (1997). Chemistry of the Elements (2nd ed.). Butterworth-Heinemann. p. 620. ISBN 978-0-08-037941-8.
2. Baird, Christopher S. (2019). "Absorption of electromagnetic radiation". AccessScience. McGraw-Hill. doi:10.1036/1097-8542.001600. Retrieved 17 June 2023.
3. Tretkoff, Ernie (August 2005). "This Month in Physics History: Einstein Predicts Stimulated Emission". American Physical Society News. 14 (8). Retrieved 1 June 2022
4. Hecht, Jeff (2021). "Laser". Encyclopedia Britannica. Retrieved 1 June 2022.
5. Sufyan Sharafedin Mohammed (2019). Mapping Molecules in Nile Water in Northern Sudan Using Raman Spectroscopy. Sudan university of science and technology. Laser Institute.
6. Crouch, Stanley R.; Skoog, Douglas A.; Holler, F. J. (2007). Principles of instrumental analysis. Australia: Thomson Brooks/Cole. ISBN 9780495012016
7. Mariani, Z.; Strong, K.; Wolff, M.; Rowe, P.; Walden, V.; Fogal, P. F.; Duck, T.; Lesins, G.; Turner, D. S.; Cox, C.; Eloranta, E.; Drummond, J. R.; Roy, C.; Turner, D. D.; Hudak, D.; Lindenmaier, I. A. (2012). "Infrared measurements in the Arctic using two Atmospheric Emitted Radiance Interferometers". Atmospheric Measurement Techniques. 5 (2): 329–344.

ISSN: 0937-583x Volume 90, Issue 7 (July -2025)
https://musikinbayern.com **DOI https://doi.org/10.15463/gfbm-mib-2025-*418***
Bibcode:2012AMT.....5..329M. doi:10.5194/amt-5-329-2012.

8. J.M. Chalmers, H.G.M. Edwards, M.D. Hargreaves Infrared and Raman spectroscopy in forensic science (1st ed.), John Wiley & Sons Ltd., United Kingdom (2012)
9. D.A. Skoog, F.J. Holler, S.R. Crouch Principles of instrumental analysis (6th ed.), Cengage Learning (2006)
10. E. Smith, G. Dent Modern Raman spectroscopy: a practical approach John Wiley & Sons, England, Chichester (2005)

,