

PUBLISHED BY

# INTECH

open science | open minds

## World's largest Science, Technology & Medicine Open Access book publisher



**2750+**  
OPEN ACCESS BOOKS



**96,000+**  
INTERNATIONAL  
AUTHORS AND EDITORS



**88+ MILLION**  
DOWNLOADS



**BOOKS**  
DELIVERED TO  
151 COUNTRIES

AUTHORS AMONG  
**TOP 1%**  
MOST CITED SCIENTIST



**12.2%**  
AUTHORS AND EDITORS  
FROM TOP 500 UNIVERSITIES



Selection of our books indexed in the  
Book Citation Index in Web of Science™  
Core Collection (BKCI)

Chapter from the book *Infrared Spectroscopy - Anharmonicity of Biomolecules, Crosslinking of Biopolymers, Food Quality and Medical Applications*

Downloaded from: <http://www.intechopen.com/books/infrared-spectroscopy-anharmonicity-of-biomolecules-crosslinking-of-biopolymers-food-quality-and-medical-applications>

Interested in publishing with InTechOpen?  
Contact us at [book.department@intechopen.com](mailto:book.department@intechopen.com)

---

## Introduction to the Book

---

Theophile Theophanides

Additional information is available at the end of the chapter

<http://dx.doi.org/10.5772/60123>

---

Infrared (IR) Spectroscopy is the most used tool today for the characterization and identification of materials, and biomaterials. In the last 20 years, its applications have been extended to large biological materials, such as proteins, DNA and membranes [1] and to healthy or diseased human tissue (e.g. cancer, atheromatic plaques, etc) [2, 3]. The technique is extensively used not only for organic compounds but almost all substances and is popular because it is simple, easy to perform, accurate and cost effective. It is hoped that in the very near future, affordable small IR instruments will be build to assist in fast pre-diagnosis and diagnosis, in clinical settings.

Functional groups like  $-CH_2$ ,  $-CH_3$ ,  $-NH$ ,  $-OH$ , etc are easily identified from an IR spectrum and the material and biomaterial that contains them can be detected and conveniently compared with library spectra. Modern Fourier Transform Infrared (FT-IR) Spectrometers, can obtain an average of 100 to 150 spectra in the mid-infrared region, in a few seconds and with excellent resolution, a vast improvement from the past. FT-IR Spectrometers are now available at low cost (~€40,000) for the analytical chemist and the structural chemical spectroscopist. [4].

The aim of this book is to assist the chemist, spectroscopist and any other scientist interested in applying FT-IR. Presented herein are signature bands at high frequency regions ( $4,000-1,500\text{ cm}^{-1}$ ), capable of giving structural information [5-10]. The positions and intensities of the absorption bands can be used to characterize a compound from library spectra and to confirm the presence of a particular group in order to obtain information as to the structure and conformation of the molecule and its microenvironment. Skeletal vibrations of molecules ( $1,500-400\text{ cm}^{-1}$ ) can change substantially with conformational changes. However these should be used with caution and cannot be applied with a high degree of confidence to structural modifications taking place to large biomolecules. It is in assisting the IR spectroscopist in determining with confidence any particular identification and characterization of a molecule from "signature bands", that this monograph aims to be of value.

## Author details

Theophile Theophanides

Emeritus Professor of NTUA

## References

- [1] Theophanides, T, Angiboust, J.P. Manfait, M.In.:Spectroscopic and Structural Studies of Biomaterials, I. Proteins, ed., Twardowski, Sigma Press, Wilmslow, UK, p. 3 (1988).
- [2] Theophanides,T. (1984), *Fourier Transform Infrared Spectroscopy*, D. Reidel Publishing Co. Dodrecht,The Netherlands.
- [3] Theophanides, T.&Rizzarelli, E. (1991).*Chemistry and Properties of Biomolecular Systems, Topics in Molecular Organisation and Engineering*, Kluwer Academic Publishers, Dodrecht, The Netherlands.
- [4] Theophanides, T.,Anastassopoulou,J.& Fotopoulos,N. (1997).*Fifth International Conference on the Spectroscopy of Biological Molecules*, Kluwer Academic Publishers, Dordrecht,The Netherlands.
- [5] Theophanides, T. (2012).*Infrared Spectroscopy-Life and Biomedical Sciences*, Vol.I InTech, open science.
- [6] Theophanides, T. (2012).*Infrared Spectroscopy Materials Science, Engineering and Technology*, Vol. II, InTech open science.
- [7] Petra, M. Anastassopoulou, J.Theologis, T. &Theophanides, T.(2005) Synchrotron micro-FT-IR spectroscopic evaluation of normal paediatric human bone, *J. Mol Structure*, Vo 733, pp. 101-110.
- [8] L.J. Bellamy, *The Infrared Spectra of Complex Molecules*, Wiley, New York, 1958
- [9] Goormaghtigh E, Raussens V, Ruyschaert JM, Attenuated total reflection infrared spectroscopy of proteins and lipids in biological membranes, *Biochim Biophys Acta*, 1999 Jul 6;1422(2):105-85.
- [10] Ferraro JR, Basile L.*Fourier Transform Infrared Spectroscopy*,Academic Press, 1979, New York.