Krzysztof Bec
Christian Huck *Editors*

Proceedings of the 21st International Conference on Near Infrared Spectroscopy

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Preface

The 21st meeting of the International Council of Near Infrared Spectroscopy (ICNIRS), NIR 2023, was held from August 20 to 24, 2023, at the Congress Innsbruck in Austria. This event marked a significant return to in-person gatherings after the disruptions caused by the COVID-19 pandemic. As the key biennial event for the global NIR spectroscopy community, NIR 2023 continued the best traditions established by previous meetings. The global nature of this event was evident in both the diversity of participants and the breadth of topics covered.

The conference motto, "Good Vibrations, Smooth Contours," encapsulated the harmony of scientific excellence, a stimulating atmosphere, and personal connections—the key elements that the chairman, organizing committee, and all those involved in the organization of NIR 2023 aimed to achieve. The program was diverse, spanning from the fundamentals of spectroscopy to the latest methodological and technological advances, demonstrating the immense potential and wide-ranging applications of NIR spectroscopy. Equally important, however, were the personal interactions and networking opportunities that NIR 2023 facilitated.

Taking place in the challenging post-lockdown circumstances, the success of NIR 2023 would not have been possible without the contributions of various parties. On behalf of the organizing committee, we would like to extend our sincere gratitude to the Austrian Society for Analytical Chemistry (ASAC) and Die Österreichische Chemische Gesellschaft (GöCH) for hosting the event. We also acknowledge the tireless efforts of the scientific committee, the Best Poster Award (BPA) committee, and the session chairs, as well as the exceptional support provided by the Congress Messe Innsbruck team. Special thanks goes to the students from the Institute of Analytical Chemistry at the University of Innsbruck for their outstanding assistance and commitment during the conference.

We are deeply grateful to our sponsors, whose generous support was essential for the success of the event. NIR 2023 was significantly enriched by the participation of our exhibitors, whose contributions enhanced the conference experience and was met with keen interest among the participants.

Last but not least, our heartfelt appreciation goes to all the participants, speakers, and poster presenters at NIR 2023. Your dedication and contributions to the NIR community made this event truly memorable. Special recognition is also due to the contributors to the NIR 2023 Proceedings volume, whose continued dedication to the event and the community is remarkable.

We believe that together we have advanced the progress of NIR spectroscopy, contributing to its ongoing success in analytical chemistry. Thank you for being part of NIR 2023 in Innsbruck.

On behalf of the NIR 2023 Organizing Committee, Editors of The proceedings of 21st International Conference on Near Infrared Spectroscopy

Innsbruck, Austria

Krzysztof Bec
Christian Huck

Organization of NIR 2023

The 21st meeting of the International Council of Near Infrared Spectroscopy (ICNIRS)

Conference Chairperson

Christian Huck

Consultant

Wolfgang Lindner

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Satoru Tsuchikawa

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Good Vibrations, Smooth Contours: NIR 2023 Conference in Hindsight

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Abstract. NIR 2023, the 21st meeting of the International Council of Near Infrared Spectroscopy (ICNIRS), took place from August 20–24, 2023, in Innsbruck, Austria. This was the first time ICNIRS was held in Austria, and with over 380 participants from 37 countries, this gathering marked a strong return to in-person events after the disruptions caused by COVID-19. As the top global conference in the area of NIR spectroscopy, its success confirmed the continuously evolving nature and growing importance of the technique and its applications.

1 Conference Recap

NIR 2023, the 21st meeting of the International Council of Near Infrared Spectroscopy (ICNIRS), took place from August 20–24, 2023, in Innsbruck, Austria. This was the first time ICNIRS was held in Austria, and with over 380 participants from 37 countries, this gathering marked a strong return to in-person events after the disruptions caused by COVID-19. As the top global conference in the area of NIR spectroscopy, its success confirmed the continuously evolving nature and growing importance of the technique and its applications.

This technical article provides a hindsight on the gathering, with the aim of giving the readers of the Conference Proceedings a good overview of the event. NIR 2023 featured a diverse program that included everything from the basics of spectroscopy to the latest advances in methods and sensor technology. Besides the plenary, award, and keynote speeches, the symposium included six outstanding workshops, numerous oral presentations, a vivid moderated discussion, poster sessions, social events, and lots of networking opportunities in the scenic heart of the Alps (Fig. 1). The conference presentations reflected the newest trends in developing methods and instrumentation and highlighted the evolving field of practical applications of NIR spectroscopy in various industries, spanning from agriculture, through food safety, medical applications, pharma, to environmental monitoring, just to name a few. The technical program was complemented by an exhibition with leading vendors showcasing the latest technology and solutions in the field.

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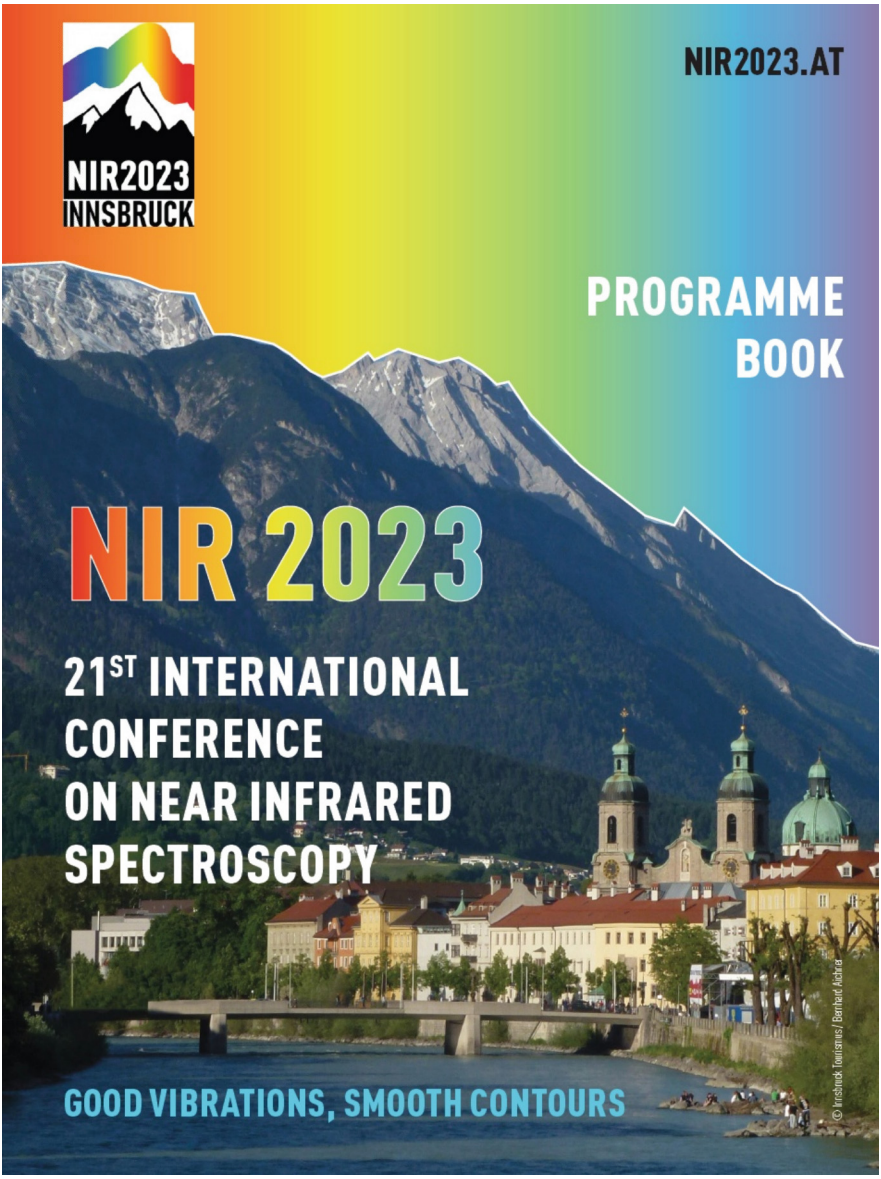

Fig. 1. The banner motif of NIR 2023, the 21st meeting of International Council of Near Infrared Spectroscopy (August 20–24, 2023, Innsbruck, Austria) as seen on the front cover of the Program Book.

2 Participants

The event in Innsbruck proved to be a vibrant gathering of the NIR community, where experts, academics, and industry professionals met together to exchange knowledge and stimulate future progress in the field. NIR 2023 brought together 386 participants from 37 countries around the world (Fig. 2). Among the presenting authors (286 abstracts), 25 were plenary, keynote, or award lectures. The remaining presentations included 79 oral presentations, 25 engaging flash talks, and 157 posters. Six specialized workshops attracted 178 participants who received in-depth training on various topics (details in Sect. 3.1). The conference dinner was a highlight, bringing together over 300 people for an outstanding evening. These statistics show the enthusiastic reception of NIR 2023 within the global NIR community, reflecting the growing momentum and international reach of NIR spectroscopy.

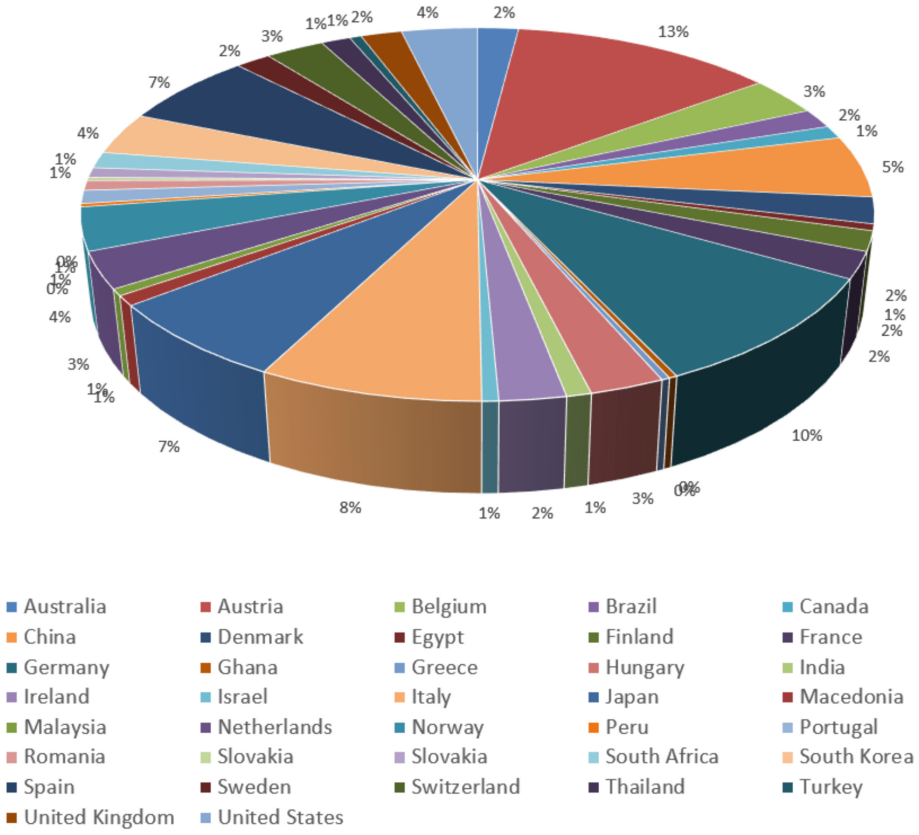

Fig. 2. Geographical distribution of delegates in percentage (legend aligns row-wise with the pie chart; countries listed alphabetically).

3 A Glimpse into the Scientific Content

Following the Opening Ceremony on Sunday, August 20th, the NIR 2023 Technical Program in the conference in the following days consisted of morning plenary and award lectures, followed by parallel afternoon sessions (Fig. 3). This structure offered a diverse experience and accommodated multiple thematic sessions, each reflecting current research activities and application trends in the field. The opening day also included a suite of workshops. The following sections present basic details on the key elements of the conference program.

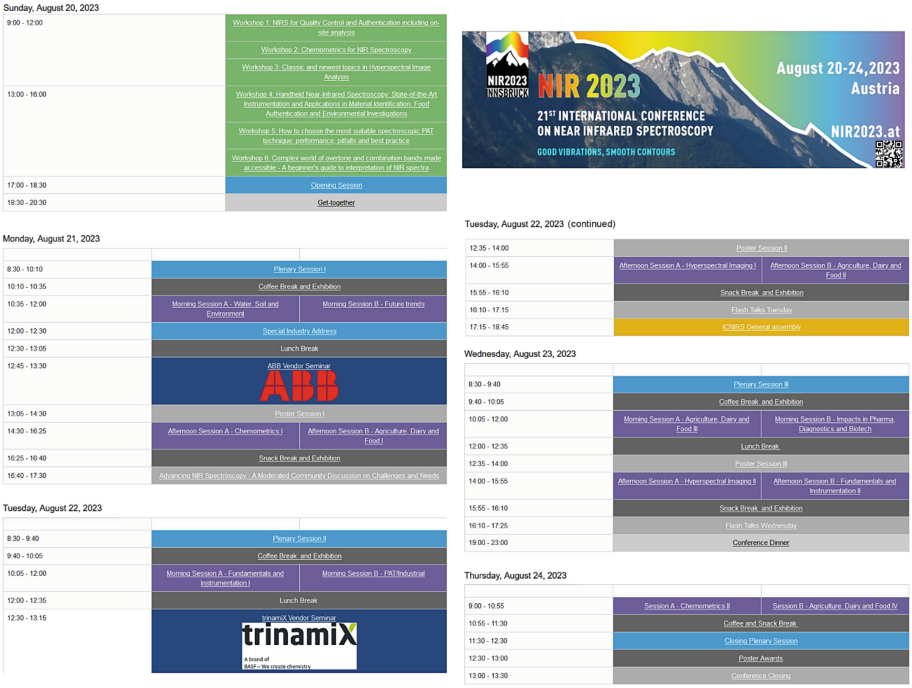

Fig. 3. The technical program of NIR 2023 conference.

The scope of topics presented at NIR 2023 reflected the dynamic nature and diverse contexts in which NIR spectroscopy is applied in modern science and industry (Fig. 3). NIR 2023 served as a strong indicator of trends in near-infrared spectroscopy and its applications. This technique has emerged as a powerful analytical tool, making invaluable contributions in various applications. In recent decades, marked by agricultural challenges and repeated major food safety incidents, it has become a key asset in the agri-food sector efforts to maintain food sustainability, safety, and quality. This significance was well represented in the conference themes (Fig. 4).

A significant focus of the community was directed at methodology, with prime attention given to chemometrics, the backbone of NIR spectroscopy. Long-standing concerns about good practices in analytical NIR—such as proper sampling design and execution, the knowledgeable use of chemometrics, and the limited trust in statistical metrics of calibration models (highlighting that raw statistics should not be the sole criteria for assessing model quality, but rather considered within a broader context)—were addressed in several notable disseminations. Many presentations discussed practical aspects of this technique in industrial settings, with dedicated themes "Impacts in Pharma, Diagnostics, and Biotechnology" and "PAT/Industrial Applications". Hyperspectral imaging based on NIR spectroscopy, a powerful technique with unique potential in both basic research and applications, also featured prominently among the conference topics. Furthermore, fundamental science in areas underlying NIR spectroscopy, along with technological advancements related to sensor development, are indispensable for the continued progress of the field; this topic significantly contributed to the scientific scope of the meeting (Fig. 4).

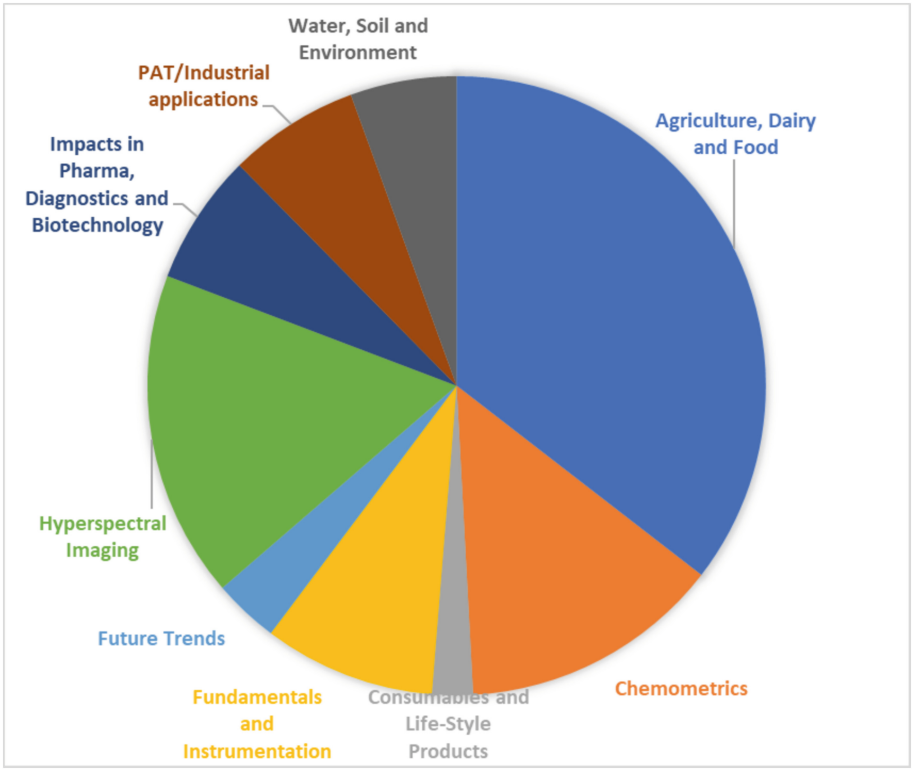

Fig. 4. The scope of topics presented at NIR 2023. Chart area represents the number of abstracts in each theme.

At the same time, the NIR community remains attentive to the ongoing limitations and emerging challenges in the field. These aspects received special attention during the Moderated Community Discussion, which focused on key issues to be resolved, such as low sensitivity, subpar chemical specificity (or selectivity); and the increasing need for smoother integration of NIR spectroscopy with other analytical chemistry techniques, particularly in demanding scenarios like process analytical technology (PAT) in the pharmaceutical industry.

During the discussion, concerns were also raised about the rapidly growing application of contemporary artificial intelligence (AI) methods, including deep learning techniques, which, if used extensively, could promote the 'black box' usage of NIR spectroscopy. This concern resonated throughout the NIR 2023 Conference, not only during the Moderated Community Discussion but also in several presentations. The community is actively addressing these challenges and emerging issues to continue advancing NIR spectroscopy as a mature analytical technique capable of adopting new concepts in reliable manner. Coincidentally, the transformative role of NIR spectroscopy in analytical chemistry and practical applications was reflected in the theme "Future Trends", as well as in emerging topics such as "Consumables and Lifestyle Products".

3.1 Pre-Conference Workshops

NIR 2023 featured a comprehensive array of workshops led by distinguished experts in their respective fields. These workshops were designed to provide participants with solid training and key know-how, allowing them to deepen their understanding and enhance their expertise in near-infrared spectroscopy.

- **Handheld Near-Infrared spectroscopy**. This workshop, led by Hui Yan and Heinz W. Siesler, explored the rapid advancements in handheld NIR spectrometers. It offered an overview of current instrumental developments and practical applications in fields such as material control, food authentication, and environmental investigations. The workshop also included a practical part, the hands-on experiments with miniaturized NIR spectrometers, making it attractive to a wide audience.
- **Interpretation of NIR spectra**. Led by Krzysztof Bec and Justyna Grabska, this workshop addressed the physical complexities of NIR spectra and the key problem of interpretation. It provided insights into how to accurately dissect NIR spectral lineshape and also dispelled common myths and misconceptions. The workshop was prepared for both beginners and experienced professionals, offering a clear and comprehensive format for understanding NIR spectroscopy.
- **Spectroscopic Process Analytical Technology (PAT)**. Led by Rudolf Kessler and Waltraud Kessler, this workshop covered the basics of PAT with a focus on optical spectroscopy. It included discussions on representative sampling, robustness, and practical applications. Participants gained know-how essential for the sector and good understanding of the role of PAT in smart production and its potential for molecular-level process control.
- **Chemometrics for NIR spectroscopy**. This workshop was led by Tom Fearn, a distinguished expert in chemometrics, mathematics and statistics. The workshop explored the fundamental concepts of creating and validating quantitative and qualitative NIR

spectroscopic calibrations using chemometrics. Topics ranged from choosing a training set to measures of performance and validation of chemometric models, i.e., the critical aspect of any application of NIR spectroscopy.

- **On-site NIRS for quality control and authentication**. Conducted by Dolores Pérez-Marín, this workshop focused on practical aspects of on-site NIRS applications for quality control and authentication, in particular in the essential agri-food applications. Participants learned about instrumentation options, sampling, calibration, and the development of predictive models. Real-world examples of on-site NIRS applications were also discussed.
- **Hyperspectral image analysis**. Led by José Manuel Amigo, this workshop offered a hands-on experience in hyperspectral image analysis. It covered spatial and spectral preprocessing, classical data mining methods, spectral unmixing, library search, target anomaly detection, and classification. Participants had the opportunity to work with dedicated examples and exercises using MATLAB and HYPER-Tools.

These workshops were met with a remarkable interest, with impressive 178 delegates registered in total. Notably, many participants signed up for multiple workshops, further confirming great interest in the community for exploring new aspects of NIR spectroscopy.

3.2 Plenary Sessions

The morning Plenary Sessions on the first three days of the conference began with Award Ceremonies. Thus, throughout most of the event, attendees had the distinct privilege of starting their day with outstanding presentations delivered by leaders in their respective fields. Well-deserved recognition was given to Harald Martens, who received the Karl Norris (KN) Award; Wouter Saeys, the recipient of the Tomas Hirschfeld (TH) Award for 2022; and Roger Meder, who was honored with the Tomas Hirschfeld Award for 2023.

The KN Awardee, **Harald Martens**, from the Norwegian University of Science and Technology NTNU, presented "Hybrid Subspace Modelling: Linking Multivariate Regression and Explainable AI" on Monday, 21st August. He discussed using chemometric multivariate calibration for selectivity enhancement, which requires less calibration data and offers insight into causality. He also explored AI and deep learning, which demand more data but provide flexibility. The lecture focused on when to use each approach for handling high-speed spectroscopy data, emphasizing the transformation of raw spectra into linear quantifications.

Wouter Saeys, from KU Leuven Department of Biosystems in Leuven, Belgium, delivered his TS Award Lecture titled "Dealing with Light Scattering in NIR Spectroscopy: Remove or Exploit?" on Tuesday, 22nd August. He explored the complexities of dealing with light scattering in NIR spectroscopy, especially in turbid media. While traditional empirical scatter correction methods have their merits, Wouter Saeys introduced a novel approach. By combining multiple diffuse reflectance and/or transmittance measurements with light propagation models, he demonstrated how to separate the effects of light absorption and scattering. This innovative technique promises more reliable estimations of chemical composition and provides valuable insights into microstructural

properties, making it a breakthrough in various applications, particularly in the agrifood domain.

Roger Meder, representing Ridley Agriproducts, Meder Consulting, and the University of the Sunshine Coast, delivered the TS award presentation on Wednesday, 23rd August. With a career spanning 30 years, he shared insights gained from long practice in analytical spectroscopy. Three key lessons emerged: the importance of finding mentors from diverse fields, the value of asking deep questions, and the necessity of solving interdisciplinary problems. His presentation emphasized the need for multidisciplinary collaboration in addressing contemporary challenges.

The Award Ceremonies and associated lectures were followed by a prestigious lineup of plenary speakers who shared insights into diverse applications of NIR spectroscopy. The Plenary Lectures at NIR 2023 featured the addresses from the following leaders in the field.

Gerhard Litscher (Medical University of Graz, Austria), in the first opening Plenary Lecture on Sunday afternoon, 20th August, presented the role of NIR spectroscopy in medicine, linking its advantages well-known in analytical applications with its potential in biomedical studies and clinical practice.

Boris Mizaikoff (University of Ulm, Germany) followed with the subsequent opening Plenary Lecture, in which he explored the world of gas sensors during his lecture. He focused on sensors based on solid-state waveguides, showcasing the advantages of both NIR and FT-IR (i.e., MIR) techniques. By combining these approaches, he highlighted the potential for more effective gas sensing.

Heinz Siesler (University of Duisburg-Essen, Germany) kicked off Monday morning session by drawing on his extensive experience in vibrational spectroscopy, including his pioneering work with NIR spectroscopy at Bayer in the late 1970s and early 1980s. He emphasized the versatility of the technique while candidly addressing the enduring challenges NIR spectroscopy has faced since its inception, some of which continue to persist despite significant changes in its application landscape.

Michael Popp (CEO, Bionorica, Neumarkt, Germany): his presentation titled "NIRvolution" discussed the background and current frontier of development of phytopharmaceutical applications of NIR spectroscopy in Bionorica, in cooperation with Institute of Analytical Chemistry of the University of Innsbruck.

Søren Engelsen (University of Copenhagen, Denmark) enriched the audience with his talk on how NIR spectroscopy meets green chemistry. Drawing from his extensive experience in both teaching and research, he shed light on the symbiotic relationship between green chemistry initiatives and NIR technology, emphasizing its pivotal role in contemporary projects. Furthermore, his insights into industrial applications and perspectives as the President of ICNIRS added invaluable depth to his lecture, offering a perspective view of the current NIR spectroscopy in practical terms.

Marena Manley (University of Stellenbosch, South Africa) took attendees on a journey that began on August 1st, 1975. She explored the fascinating realm of cereal quality analysis using NIR spectroscopy, showcasing her decades-long experience in this field. Her presentation shed light on the enduring relevance and practicality of NIR spectroscopy in the assessment of cereal quality.

Yukihiro Ozaki (Kwansei-Gakuin University, Japan) delivered an illuminating presentation on the latest advancements in NIR imaging techniques. His lecture presented innovative applications and technological breakthroughs in this area. By sharing cutting-edge developments in this field, he provided valuable insights into the exciting future of NIR imaging technology.

Federico Marini (University La Sapienza, Rome, Italy) explored the role of chemometrics, the backbone of NIR spectroscopy, focusing on key new promising developments in this critically important area. Chemometrics and spectroscopy work hand in hand, highlighting that it is only the combination of these elements that makes NIR an effective and versatile analytical method.

3.3 Moderated Community Discussion

Special attention should be given to the Moderated Community Discussion, a key event at NIR 2023. It provided a forum where experts, researchers, practitioners, and industry leaders came together to address the challenges and explore new developments in NIR spectroscopy. Moderated by well-known experts Heinz Siesler, Rudolf Kessler, and Tom Fearn, this interactive session sparked lively discussions and knowledge exchanges among participants.

The discussion developed spontaneously and covered a wide range of topics, including ways to overcome the limitations of NIR spectroscopy, new applications, and the future direction of the field. Participants engaged in dynamic conversations about the evolving landscape of NIR spectroscopy. In particular, the session featured in-depth conversations on several critical topics:

- **Overcoming inherent limitations**. The discussion focused on the ongoing challenges associated with NIR spectroscopy, including long-standing limitations related to sensitivity and chemical specificity. Various ideas of improving the technique in these regards were mentioned, including the prospects for reliable application of the concept of surface-enhancement effect in NIR spectroscopy.
- **Integration with other analytical techniques**. There was a strong emphasis on the need for better integration of NIR spectroscopy with other analytical methods, especially in complex scenarios like process analytical technology (PAT) in the pharmaceutical industry. The goal is to enhance the technique in its effectiveness and versatility by combining it with complementary technologies.
- **Advancements in chemometrics**. The discussion highlighted recent advancements in chemometrics, the analytical backbone of NIR spectroscopy. Participants explored new developments that enhance the data analysis capabilities, addressing how improved chemometric methods can mitigate some of the limitations of NIR spectroscopy.

- **Artificial intelligence and deep learning**. The community raised concerns about the application of artificial intelligence (AI) and machine learning, including deep learning techniques, in NIR spectroscopy. There was debate about the risks of these technologies leading to 'black box' scenarios where the decision-making process of models becomes opaque. The need for transparent and interpretable AI methods and their well-informed application was emphasized.
- **Future applications and trends**. The discussion also touched the emerging applications of NIR spectroscopy, including its potential in new sectors and innovative uses. Participants discussed how the technique can be adapted to meet the evolving needs of individual industries and research fields.
- **Communication and collaboration**. The moderated discussion acknowledged the importance of improving communication and collaboration with other analytical chemistry communities. Enhancing cross-disciplinary interactions is crucial for advancing the field and applying NIR spectroscopy in new and diverse contexts.

Effectively, the Moderated Discussion highlighted the dedication of the conference delegates to helping the wide community of NIR practitioners to take advantage of new opportunities in a better-informed manner.

3.4 Oral Sessions and Flash Talk Sessions

The majority of the following disseminations took place throughout the parallel oral sessions, each focused on distinct aspects of NIR spectroscopy. These sessions were organized to cover several specific topics and reflect the main areas of activity in the field. The thematic areas covered in the oral sessions were as follows.

- **Monday** (21st August); the discussions began with a focus on "Water, Soil, and Environment," followed by an exploration of "Future Trends" in NIR spectroscopy. The day also included sessions on "Chemometrics I" and "Agriculture, Dairy, and Food I."
- **Tuesday** (22nd August); the second day featured sessions on "Fundamentals and Instrumentation I," "Process Analytical Technology (PAT)/Industrial Applications," "Hyperspectral Imaging I," and "Agriculture, Dairy, and Food II."
- **Wednesday** (23rd August); midweek, the discussions continued with sessions dedicated to "Agriculture, Dairy, and Food III," "Impacts in Pharma, Diagnostics, and Biotechnology," "Hyperspectral Imaging II," and "Fundamentals and Instrumentation II."
- **Thursday** (24th August); the final day of oral sessions included "Chemometrics II" and "Agriculture, Dairy, and Food IV."

Despite the tight schedule, NIR 2023 included two Flash Talk Sessions, held on Tuesday and Wednesday. Each session featured around 25 speakers, each allotted 5 min for their presentation. Discussions (Q&A) followed the final presentation of each session. The Flash Talk Sessions were met with great interest from the conference participants, with considerably positive feedback from both the presenters and the audience.

3.5 Posters Presented at NIR 2023 and the Best Poster Awards

The poster sessions at NIR 2023 were another testament to the dedication of NIR community. A total of 157 posters were presented, covering a wide spectrum of topics and research areas. Each poster was a unique contribution to the conference; preparing and presenting a poster is a considerable commitment, requiring effort, dedication, and a touch of artistry in design. Therefore, the Conference placed particular focus on commemorating the poster presenters and their co-authors in the form of Best Poster Award (BPA) competition.

The prizes in the BPA competition, were sponsored by Shimadzu (prize pool of 3000 EUR in total, with the main prize of 1000 EUR) and Springer (book voucher, 300 EUR in value). The poster evaluation committee, consisting of Krzysztof Bec (coordinator/chair), Jose Manuel Amigo, Vincent Baeten, Hoeil Chung, Cristina Malegori, Marena Manley, Longhai Guo, Zoltan Kovacs, Dolores Pérez-Marin, Heinz Siesler, and Satoru Tsuchikawa, carefully evaluated the posters. The criteria in particular considered in the evaluation procedure included scientific excellence, clarity and quality of presentation and the discussion at the poster, each of equal importance for the final score of the poster.

Approximately 100 participants took part in the BPA competition. **The winners** of the main prizes in the BPA competition at NIR 2023, are as follows (here, the presenting authors listed only).

- **First Prize**: Valeria Fonseca Diaz (Software Competence Center Hagenberg, Austria) for "Interpretable and Interactive Transfer Learning in Process Analytical Technology."
- **Second Prize**: Irina Benson (Noaa Fisheries / Afsc, United States) for "The future of fish age estimation: deep machine learning coupled with Fourier transform near infrared spectroscopy of otoliths."
- **Third Prize**: Alissa Drees (University Of Hamburg, Germany) for "Rapid Determination of Nutmeg Shell Content in Ground Nutmeg using FT-NIR Spectroscopy and Machine Learning."
- **Recognition Prizes** sponsored by Shimazdzu were awarded to: Nicola Cavallini (Italy), Haeun Kim (South Korea), Nicholas Davison (United Kingdom), Don van Elst (Netherlands), Adham Hamed (Egypt), Erik Tengstrand (Norway), Ingunn Burud (Norway), Alejandra Arroyo-Cerezo (Spain), Chayanid Sringarm (Thailand). An additional **Recognition Prize** sponsored by Springer was awarded to Maria C. Hespanhol (Brazil).

While not awarded with prizes, the following posters and their presenters as well as the respective co-authors also distinguished themselves among others. They were called to the podium as the **Nominees** during the BPA Ceremony on Friday, and recognized for their valuable contributions to the field:

Celio Pasquini (State University Of Campinas, Brazil), Alejandra Arroyo-Cerezo (University of Granada, Spain), Chayanid Sringarm (Naresuan University, Thailand), Don van Elst (Eindhoven University Of Technology, Netherlands), Adham Hamed (Si-ware Inc., Egypt), Erik Tengstrand (Nofima, Norway), Ingunn Burud (Norwegian University of Life Sciences, Norway).

Congratulations to the Winners and the Nominees, and thank you to all the 157 poster presenters and their co-authors for sharing their research and enriching the poster sessions.

4 Conference Host, Organizers, and Committees

As the Chair of this event acted Christian Huck from the University of Innsbruck, Austria; the Head of the Institute of Analytical Chemistry. The conference was hosted by the Austrian Society for Analytical Chemistry (ASAC) in cooperation with Die Österreichische Chemische Gesellschaft (GöCH), emphasizing the key role of NIR spectroscopy in the landscape of modern analytical chemistry.

The Organizing Committee for NIR 2023 was responsible for the organization and management of the conference. In this duty, the Chairman of the conference, Christian Huck, was supported by Wolfgang Lindner (University of Vienna, Austria), the Honorary President of ASAC, who brought his experience in organization of major symposia and acted as the Consultant on behalf of the host. The following members of the Organizing Committee included Krzysztof Bec, Justyna Grabska, and Matthias Rainer, all from the University of Innsbruck, Austria.

The Scientific Committee for NIR 2023 was composed of a distinguished group of experts from various institutions and countries. This committee played a crucial role in maintaining the scientific rigor and excellence of the conference. The members of the committee included (listed alphabetically) Günther K. Bonn (University of Innsbruck, Austria and ADSI-Austrian Drug Screening Institute), Nanning Cao (CNIRS and Ardent Mills, USA), Miroslaw Czarnecki (University of Wrocław, Poland), Søren Balling Engelsen (University of Copenhagen, Denmark), Ana Garrido-Varo (University of Cordoba, Spain), Longhai Guo (Beijing University, China), Christian Huck (University of Innsbruck, Austria), Zoltán Kovács (Hungarian University of Agriculture and Life Sciences, Hungary), Wolfgang Lindner (University of Vienna, Austria), Marena Manley (University of Stellenbosch, South Africa), Roger Meder (Meder Consulting, Australia), Boris Mizaikoff (University of Ulm, Germany), Yukihiro Ozaki (Kwansei Gakuin University, Japan), Celio Pasquini (University of Campinas, Brazil), Heinz Siesler (University of Duisburg-Essen, Germany), Roumiana Tsenkova (Kobe University, Japan), and Satoru Tsuchikawa (Nagoya University, Japan).

5 Sponsorship and Exhibition

NIR 2023 featured an outstanding exhibition of prominent vendors specializing in spectroscopy, instrumentation, chemometrics, data-science and associated software development, as well as analytical applications. This exhibition provided attendees with a unique opportunity to connect to the technological leaders in the field, explore cutting-edge technologies, innovative solutions, and the latest advancements in spectroscopic instruments and accessories, offering practical summary of the industry offerings.

While all the Sponsors and Exhibitors made valuable contributions, special recognition is reserved for the Gold, Silver and Bronze Sponsors. Bruker, the Gold Sponsor, stands as a renowned provider of scientific instruments and solutions, with a prominent presence in both basic and applied spectroscopy. Bruker's generous support vividly demonstrated their commitment to propelling innovation and excellence within the realm of analytical sciences. The pivotal roles of the Silver Sponsors, KAX Group, ABB, Trinamix, AB Vista, and Bionorica further enriched the conference. Their support not only bolstered the event but also underscored the collective commitment to advancing NIR spectroscopy and its applications. The conference also extends its heartfelt gratitude to several Bronze Sponsors; PerkinElmer, Shimadzu, Metrohm, Zeiss, NeoSpectra by SiWare, VIAVI Solutions, and Senorics, whose contributions were instrumental in ensuring NIR 2023 distinction. This suite of Sponsors was reinforced by Handl Tyrol, LGGC, JCNIRS, Prediktera, Elsevier, Springer, ASAC, GöCH and GDCh. A collective information on the Sponsors who supported NIR 2023 can be found on the website: https://www.nir2023.at/index.php/sponsors-exhibitors/nir-2023-sponsors-exhibitors).

6 A Vibrant Gathering: Location, Venue, Social Events, and Late Evening Networking at NIR 2023

NIR 2023 took place in Innsbruck, the capital of Tyrol. This was the first time the NIR symposium series was held in Austria, offering a mix of science, tradition, and Alpine scenery (Fig. 5). Innsbruck rich heritage and lively atmosphere created a great environment for networking and scientific exchange. The city, known as "the heart of the Alps," provided a central location that was easy to access. The Congress Innsbruck, located near the center in the Old Town, was ideal venue for the event as Delegates enjoyed exploring the city's landmarks.

Outside the venue, Innsbruck offered a range of attractions, including historical sites and outdoor activities. The nearby cable car station provided quick access to the Nordkette, reaching the Hafelekarspitze at 2334 m above sea level in just a few minutes. From the top, delegates enjoyed breathtaking panoramic views of the surrounding Alpine peaks. Innsbruck itself boasts a charming Old Town, where visitors can explore landmarks like the Golden Roof (Goldenes Dachl), a symbol of the city with its ornate, gilded balcony. The Imperial Palace (Hofburg) offers a glimpse into the city's royal past, and the 16th-century Ambras Castle features an impressive collection of art and armor. During the summer, the city is lively with outdoor activities. Delegates could take leisurely strolls along the River Inn, enjoy the scenic parks, or visit the colorful local markets. Innsbruck's numerous cafes and restaurants provided opportunities to savor Tyrolean cuisine while soaking in the vibrant city atmosphere. Overall, the feedback on the conference and Innsbruck itself was very positive. Many delegates appreciated the socializing and networking opportunities in the city's restaurants.

We hope that the choice of Innsbruck for the 21st meeting of the International Council of Near Infrared Spectroscopy (ICNIRS) contributed positively to the conference experience and left attendees with memorable and enjoyable moments.

7 The Proceedings of NIR 2023

This volume collects around 30 selected papers associated with the Award, Plenary, Keynote as well as regular presentations disseminated at NIR 2023 Conference. Thus, the volume covers a broad array of topics that reflect the diverse and dynamic nature of NIR spectroscopy. From fundamental studies exploring the theoretical aspects of NIR to innovative applications across industries such as pharmaceuticals, agriculture, food science, and environmental monitoring, the Proceedings offer a comprehensive snapshot of the current state of the field. In addition to original research, the NIR 2023 Proceedings include perspective reviews and important communications that provide invaluable insights into emerging trends, technological advancements, and the challenges faced by researchers and practitioners alike. These contributions not only highlight the latest breakthroughs but also provide good-practice guide to informed application of NIR spectroscopy in real-world settings, highlighting how innovations are being translated into impactful solutions in the field.

We hope that the NIR 2023 Proceedings will serve as a lasting testament to the scientific and collaborative achievements of the Conference.

Fig. 5. NIR 2023 in Innsbruck - scientific and social dynamics on the background of the Jewel of the Alps (Nordkette, bottom right).

Near Infrared Spectroscopy: A "Restless" Analytical Technique for a Multiplicity of Applications

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Abstract. This article is a highly personal assessment of the development, special features and current significance of NIR spectroscopy for quality and process control in the material and life sciences. The stunning evolution over the last five decades from hang-on to UV/VIS or MIR spectrometers via stand-alone laboratory instruments to their current use as light-fiber coupled process control tools, imaging spectrometers and miniaturized sensors in pocket-size finds few analogues in instrumental analytical chemistry. The initial organizational difficulties in implementing the NIR technique in industrial analytical laboratories are addressed as well as the gradual optimization of chemometric evaluation procedures and technical advancements that have contributed to its current importance as an analytical technique. From the perspective of a conservative spectroscopist, specific beneficial features of the NIR technique are highlighted and some myths that have unnecessarily delayed the rapid spread of the NIR technique are dispelled. The current potential of the technique for in-the-field and on-site measurements is emphasized in light of advances in miniaturization and special attention will be paid to possible applications that will allow a clientele that is not necessarily scientifically trained to solve quality control and authentication problems with this technology in everyday life. Finally, the danger is addressed not to fall into the exaggerated narrative of some direct-to-consumer companies, which has raised expectations with full-bodied promises, but has harmed the very valuable technology of NIR spectroscopy, rather than promoting its further development.

Keywords: Historical development of NIR spectroscopy · comparison with MIR spectroscopy · NIR spectroscopic process control · NIR spectroscopic imaging · miniaturization · NIR spectroscopic applications in material and life sciences · environmental investigations

1 The Early Stage of NIR Spectroscopy

My entry into NIR spectroscopy almost exactly 50 years ago as part of my industrial work at a large chemical company, was made very easy for me by my predecessor who was already working with an NIR hang-on to a UV/VIS spectrometer and one of the important analytical requirements for this company at that time: the rapid analysis of

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ethylene oxide/propylene oxide (EO/PO) copolymers for water content, OH number and EO/PO ratio. This was in fact an analytical problem that was virtually tailor-made for processing with the aid of NIR spectroscopy. The separation of the $\nu(OH) + \delta(OH)$ combination vibrations of water and organic compounds observed in the NIR in contrast to the overlap of the fundmental vibrations in the MIR range - a fact of which many NIR users are still unaware today - allowed univariate calibration even at this early stage via band area evaluation of the corresponding absorption bands (Fig. 1a/b)) of transmission spectra with a practical sample thickness of 5 mm for routine analysis. The assignment of the OH-specific absorption bands was also clearly demonstrated by disappearance of the absorption band of the organic OH functionality upon peracetylation (Fig. 1c). The additional evaluation of the band ratio of the $2x\nu(CH_3)/2x\nu(CH_2)$ bands at about 1.8 µm (5555 cm^{-1}) thus made it possible to replace three separate titration methods by recording a single NIR spectrum.

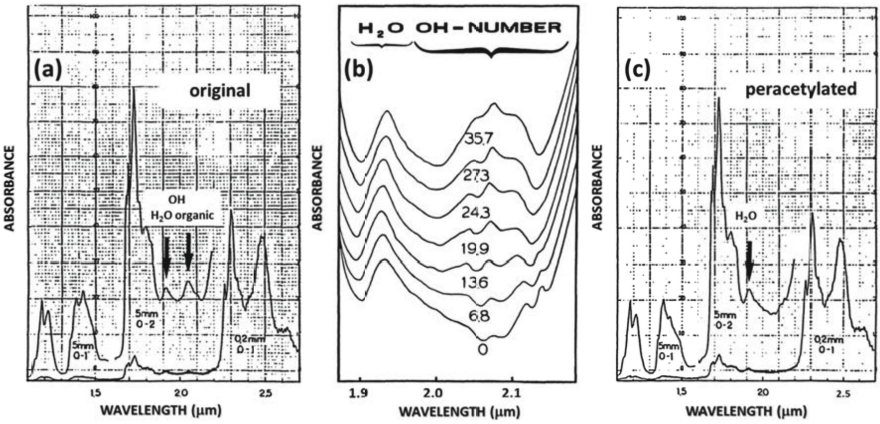

Fig. 1. NIR spectroscopic analysis of an EO/PO polyether: (a) NIR spectra of original sample at 5 mm and 0.2 mm sample thickness; (b) enlarged section of OH-specific absorption bands; (c) NIR spectra of peracetylated sample.

The availability of commercial stand-alone NIR spectrometers in combination with the first chemometric evaluation methods in the 1980s paved the way for a rapid development as an industrial quality control tool. However, delays in this process were partly due to the unexpected opposition of conservative spectroscopists to the "black-box" technique and internal problems with the billing process in analytical laboratories. It should not be forgotten that in some cases complex analytical procedures for multi-component products using various chromatographic or titration methods could be replaced by the simple recording of an NIR spectrum, resulting in major shifts in the income structure of various departments in an analytical laboratory. During this phase, however, production-related laboratories contributed significantly to the rapid further development of the method, because they only assessed the value of the technology as an extremely fast and efficient method for product analysis, irrespective of professional ethics and financial petty squabbles. Furthermore, during this phase, funding for academic projects

that focused on NIR spectroscopy was particularly poor, as the scientific and practical value of this technology had not yet been recognized by advisory committees. Only the instrumental expansion of the technique with fiber-optic coupled probes and the spread of chemometric evaluation methods for the qualitative (principal component analysis, PCA and quantitative evaluation (partial least squares, PLS) of NIR spectra gradually led to a recognition of the NIR technique that was commensurate with its practical and scientific value. In this context, I would also argue that the real luminaries of NIR spectroscopy at this time were the chemometricians, because without their input for the rapid evaluation of large NIR data sets - which were required for the various calibration procedures - the NIR technique might have remained in its infancy.

2 Myths About and Special Features of NIR Spectroscopy

At this point, it is also appropriate to dispel some myths and point out special valuable features of NIR spectroscopy. In particular, the statement and advice of conservative spectroscopists that the absorption bands in the NIR wavelength range are always broad and non-selective has been very detrimental to the initial spread of NIR spectroscopy.

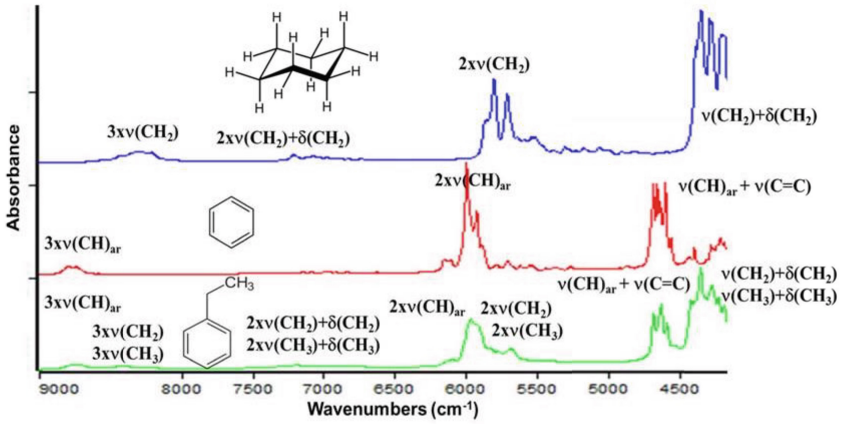

Fig. 2. NIR spectra of three organic solvents (cyclohexane, benzene, toluene) with assignment of their absorption bands.

Figure 2 shows the NIR spectra of three organic solvents, which render both arguments absurd. In fact, NIR spectra are not only selective for absorption bands of CH, OH and NH functionalities but are also characteristic for combination vibrations with C=O, C=C and other functionalities [1, 2]. Furthermore, in contrast to MIR spectroscopy, NIR spectra are not only selective but also "sample-thickness friendly", as shown in Fig. 3. This means that the wavelength range of a NIR spectrum can be selected to optimally fulfill the experimental requirements for the choice of a suitable sample layer thickness. For an on-line process control method in the petrochemical industry, for example, the short-wavelength range is preferentially selected, in which flow probes with practicable layer thicknesses in the millimeter/centimeter range can be used.

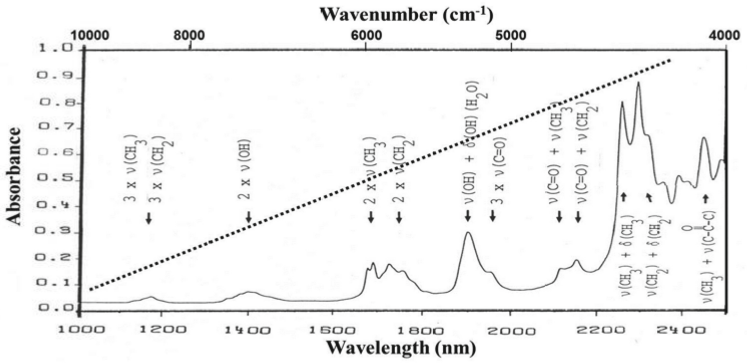

Fig. 3. NIR spectrum of methylethylketone (+5% (v/v) water) and assignment of absorption bands (the dashed line indicates the intensity decrease of higher order absorption bands).

In this context, it is of interest to mention a special spectroscopic feature: because in NIR spectroscopy it is not primarily the change in the dipole moment during the oscillation but the anharmonicity of the molecular oscillator that is the dominant factor for the occurrence of an absorption band, one of the most intense absorbers in MIR spectroscopy (poly(tetrafluoroethylene) (PTFE)) shows no absorption in the NIR spectrum. As Fig. 4 shows, the 2nd overtone of the very intense ν(CF) fundamental vibration (fluorine has an extremely high electronegativity and therefore leads to a strong dipole moment change during the C-F stretching vibration) can no longer be detected even in the MIR spectrum. PTFE is therefore used in the NIR as a non-absorbing reference material for background measurements of diffuse reflection spectra.

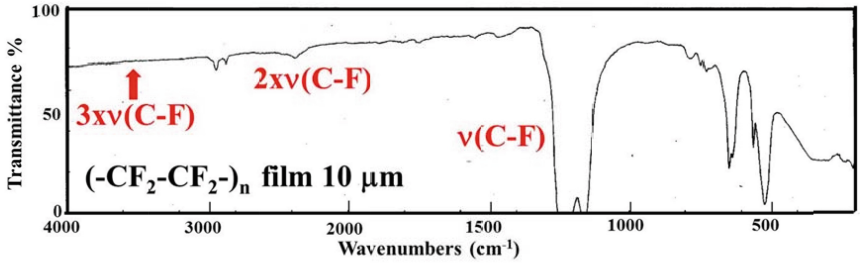

Fig. 4. MIR transmission spectrum of a 10 µm film of poly(tetrafluoroethylene) (Teflon^{TM}). The red arrow at about 3600 cm^{-1} marks the disappearance of the 2nd overtone of the very intense ν(C-F) fundamental absorption.

3 Examples of NIR Spectroscopic Process Control

Similar to the above-mentioned need for rapid analysis of EO/PO copolymers, NIR spectroscopy experienced a leap in acceptance for industrial process control in our company when we were able to demonstrate that the previously very cumbersome off-line