# Summary of Professional Accomplishments

## Katarzyna Bielska

# 1. Diplomas and scientific degrees

- MSc in physics, Nicolaus Copernicus University, 2007 supervisor: prof. dr hab. Ryszard S. Trawiński thesis: "Pressure broadening of 326.1 nm <sup>113</sup>Cd line perturbed by argon and xenon"
- PhD in physical sciences in the field of physics, Nicolaus Copernicus University, 2011 supervisor: prof. dr hab. Ryszard S. Trawiński dissertation: "Spectroscopic determination of the vapor pressure of ice"

# 2. Information on employment in research institutes or faculties/departments or school of arts

- 12.2011-09.2015: assistant, Nicolaus Copernicus University, Faculty of Physics, Astronomy and Informatics, Institute of Physics, Department of Atomic, Molecular and Optical Physics, research and teaching position
- 02.2012 09.2014: unpaid leave at the Nicolaus Copernicus University for a postdoctoral fellowship at the National Institute of Standards and Technology
- 10.2015 present: assistant professor, Nicolaus Copernicus University, Faculty of Physics, Astronomy and Informatics, Institute of Physics, Department of Atomic, Molecular and Optical Physics, research position in the period of 6 months in 2018, apart from that research and teaching position

## 3. Description of the achievements, set out in art. 219 para 1 point 2 of the Act.

## 3.1. Introduction

My long-term scientific goal is to obtain accurate models of the spectra of small molecules, such as oxygen, carbon monoxide and carbon dioxide, so that they can be effectively used in both basic research and practical applications. My research interests are focused on spectroscopy, in particular molecular spectroscopy. They include the development of experimental techniques, data analysis, and the relationship between the results of experimental and theoretical work. Among them, especially collaboration with theoretical groups which create tools for the construction of accurate spectral models. These tools, however, require thorough experimental verification in order to enable to predict spectral parameters in conditions and spectral ranges where it is currently impossible to perform high-accuracy laboratory measurements.

### 3.1.1. The importance of precise spectroscopy in atmospheric research, metrology and basic research

Spectroscopy enables remote measurements used, among others, in the study of the Earth's atmosphere and astrophysics. Observations of the Earth's atmosphere can be carried out both from satellites and from the Earth's surface, and are used to monitor its composition and parameters, and to study the ongoing processes. Interpretation of these measurements requires the use of reference data for all molecules, present in the atmosphere, that significantly contribute to absorption in a given spectral range. Then it is possible to detect molecules present in the Earth's atmosphere in trace amounts, but crucial for its condition, such as carbon monoxide or various types of pollutants. It is necessary to know all the relevant parameters of the spectral lines: not only positions

and intensities, but also line shape parameters such as pressure broadening and shifting. In addition, increasing accuracy requirements cause that the Voigt profile, which is commonly used to describe the shape of spectral lines is insufficient, and the knowledge of parameters describing more subtle effects leading to especially line narrowing and asymmetry is also needed. For this reason, both the molecules that are the main components of the atmosphere, as well as those occurring in it in trace amounts, are of interest to numerous research groups dealing with this subject.

One of the key molecules for the measurements of the atmosphere composition is the oxygen molecule. Measurements of absorption by oxygen are used, among other things, for the determination of pressure and temperature profiles in the atmosphere  $^{*1}$ , providing the basis for interpreting measurement results for other molecules. Until recently, the so-called A band, which has a spectral range of about 760 nm was mainly used in the atmospheric research. This was because it is the strongest absorption band in the red part of the oxygen spectrum and because of the lack of precise reference data for the remaining bands, in particular for the approximately 15 times weaker B band, which corresponds to a wavelength range of approximately 690 nm. It has been shown, however, that taking into account other bands apart from the A-band may significantly improve the accuracy of the obtained results. This is the case, for example, while determining the parameters of clouds, where taking into account in addition to the A band also the B band and the band originating from  $O_2 - O_2$  complexes (approx. 477 nm) reduces the uncertainty of the determined parameters by more than  $50\%^2$ . Another example of using the weaker B band of oxygen is to determine the parameters of winds<sup>3</sup> in the upper atmosphere and to monitor the presence of aerosols in the atmosphere<sup>4</sup>.

Important molecules influencing the global properties of the atmosphere are carbon monoxide and carbon dioxide. Carbon monoxide is present in the atmosphere in trace amounts, but its content is of key importance for the climate and air quality. It enters the atmosphere as a result of human emissions and biomass combustion, and is also produced by chemical reactions in the atmosphere. Its lifetime in the Earth's atmosphere is limited to weeks or months, depending on the season and altitude. Thanks to this, it is used, among others to monitor transportation processes taking place in the atmosphere<sup>5</sup>. Carbon monoxide is also involved in chemical reactions in the atmosphere that lead to the formation of greenhouse gases such as carbon dioxide and ozone, and it influences the methane content of the Earth's atmosphere, hence it is important for the study of the climate and its changes<sup>6</sup>. On the other hand, carbon dioxide strongly influences the greenhouse effect. Its content in the Earth's atmosphere is constantly growing as a result of human activity. Only between 1970 and 2010, the concentration of carbon dioxide increased by nearly  $20\%^7$ . For this reason, it is particularly important to accurately determine both the sources of carbon dioxide and the channels by which it is removed from the atmosphere. A dozen or so years ago there has been set a specific goal of monitoring the carbon dioxide content at the level of 1 ppm (*part-per-million*), which corresponds to relative standard uncertainty of about  $0.25\%^8$ . However, only recently have reference data become available, which in the future may enable the assumed accuracy of measurements in the Earth's atmosphere to be obtained<sup>9</sup>. Usually, even if sufficiently accurate data are available, they are not independently confirmed by another research group, while the scatter of results obtained in different laboratories significantly exceeds 1% of the line intensity values.

The molecules mentioned above are relatively simple as they consist of only two or three atoms. Due to their importance for the Earth's atmosphere, they are studied by many theoretical and experimental groups, but so far there are no accurate parameter values that would allow for spectral simulations. At the same time, growing expectations are emerging. Apart from the aforementioned carbon dioxide, it is not possible to monitor the carbon monoxide content. In this case, the World Meteorological Organization (WMO) recommends inter-laboratory comparisons of carbon monoxide content at 1 ppb (*part-per-billion*) level or with a relative standard uncertainty

<sup>\*</sup>References to literature in this study in the form [Hx] mean items listed in Section I of the "List of scientific achievements", while references in the form [x] denote my other publications listed in Section II.4 of this list. References to other publications have been included in the footnotes.

<sup>&</sup>lt;sup>1</sup>C. R. Nowlan et al., Journal of Quantitative Spectroscopy and Radiative Transfer 108, 371–388 (2007).

<sup>&</sup>lt;sup>2</sup>J. S. Daniel, Journal of Geophysical Research **108**, 4515 (2003).

<sup>&</sup>lt;sup>3</sup>D. A. Ortland et al., Journal of Geophysical Research: Atmospheres **101**, 10351–10363 (1996).

<sup>&</sup>lt;sup>4</sup>S. Sanghavi et al., Atmospheric Measurement Techniques **5**, 1099–1119 (2012).

<sup>&</sup>lt;sup>5</sup>J. A. Logan et al., Journal of Geophysical Research **86**, 7210 (1981).

<sup>&</sup>lt;sup>6</sup>A. Voulgarakis et al., Atmospheric Chemistry and Physics **13**, 2563–2587 (2013).

<sup>&</sup>lt;sup>7</sup>J. M. Barlow et al., Atmospheric Chemistry and Physics **15**, 13739–13758 (2015).

<sup>&</sup>lt;sup>8</sup>C. E. Miller et al., Journal of Geophysical Research Atmospheres **112**, 1–19 (2007).

<sup>&</sup>lt;sup>9</sup>D. A. Long et al., Geophysical Research Letters 47, e2019GL086344 (2020).

of  $0.5\%^{10}$  .

The above considerations focus on the outline of problems related to remote sensing in the Earth's atmosphere. The problem naturally extends to astronomical observations. Interpreting them is even more difficult than in the Earth's atmosphere due to the possibility of more diverse molecules and a much wider range of thermodynamic conditions that are beyond the current capabilities of reproducing them under laboratory conditions. One of the many examples is the study of exoplanets, in which the atmospheres of so called "hot-Jupiter" planets can reach temperatures as high as 2800 K. Despite the relatively poor quality and resolution of the spectra, their interpretation requires the knowledge of not only positions and intensities, but also other parameters of the spectral lines along with their dependence on the temperature<sup>11</sup>.

Molecular spectroscopy provides an important contribution to basic research. The obvious consequence of determining the spectral parameters is obtaining information about the energy structure of the molecule, the probability of transitions between the molecule's states and about collisions with the molecules of the perturbing gas. More advanced applications of atomic and molecular spectroscopy in basic research<sup>12</sup> are possible in case of not only the simplest molecules, but also polyatomic ones<sup>13</sup>. An example of spectroscopic contribution to basic research is the measurement of the <sup>6</sup>S–<sup>7</sup>S transition in cesium atoms, the existence of which is an evidence of parity violation<sup>14</sup>. In turn, precise spectroscopy of the hydrogen molecule and its isotopologues and ions<sup>15</sup> or weakly bound molecules<sup>16</sup>, such as Yb<sub>2</sub>, in conjunction with advanced theoretical calculations, may be an area of search for evidence for the existence of the so-called "fifth force", that is, a postulated, yet unknown interaction. On the other hand, larger molecules can be used, for example, in studies on the invariability of physical constants<sup>17</sup>. Such studies, however, usually require exceptional precision and accuracy of measurement, as well as high sensitivity of the experimental system. They significantly exceed the standard capabilities of commonly used spectrometers, being another source of motivation for the development of measurement techniques.

An important field of applications is also the use of molecular spectroscopy in metrology. It has been proposed to use spectroscopic techniques to determine new temperature<sup>18</sup> and pressure<sup>19</sup> standards, however they require knowledge of spectral line intensities with an accuracy significantly higher than currently achievable. In contrast, spectroscopic methods may currently compete with precision mass spectrometry<sup>20</sup>. It is also proposed to use the molecular transition frequencies as frequency standards<sup>21</sup>.

From the point of view of atmospheric studies, the relatively weak absorption lines and bands, which are not saturated in the long absorption path, are particularly important. This causes obvious difficulties in laboratory measurements. The stronger of these lines can be tested with long-cell Fourier spectrometers. Weaker, such as the B band of oxygen, in laboratory conditions require the extension of the absorption path, for example, by the use of high-finesse optical cavities.

In my research work so far, I have striven to develop techniques that would enable obtaining accurate parameters of the shape of spectral lines and thus accurate simulations of these spectra. My work included both the development of experimental techniques based on optical cavities, data analysis using advanced spectral line profiles, and collaboration with a theoretical computation group leading to the development of new spectral models.

<sup>17</sup>M. G. Kozlov, Physical Review A **87**, 032104 (2013).

<sup>20</sup>A. J. Fleisher et al., Nature Physics **17**, 889–893 (2021).

<sup>&</sup>lt;sup>10</sup>P. Tans and P. Zellweger, 18<sup>th</sup> WMO/IAEA meeting on carbon dioxide, other greenhouse gases and related measurement techniques (GGMT-2015), GAW Report No. 229 (World Meteorological Organization, 2016).

<sup>&</sup>lt;sup>11</sup>P. F. Bernath, Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences **372**, 20130087–10 (2014).

<sup>&</sup>lt;sup>12</sup>M. S. Safronova et al., Reviews of Modern Physics **90**, 025008 (2018).

<sup>&</sup>lt;sup>13</sup>N. R. Hutzler, Quantum Science and Technology **5**, 044011 (2020).

<sup>&</sup>lt;sup>14</sup>C. S. Wood, Science **275**, 1759–1763 (1997).

<sup>&</sup>lt;sup>15</sup>E. J. Salumbides et al., Physical Review D **87**, 112008 (2013).

<sup>&</sup>lt;sup>16</sup>M. Borkowski et al., Scientific Reports **9**, 14807 (2019).

<sup>&</sup>lt;sup>18</sup>M. P. Arroyo and R. K. Hanson, Applied Optics **32**, 6104 (1993), R. Gotti et al., Physical Review A **97**, 012512 (2018).

<sup>&</sup>lt;sup>19</sup>R. Wehr et al., Applied Optics **42**, 6595 (2003), C. Gaiser et al., Nature Physics **16**, 177–180 (2020).

<sup>&</sup>lt;sup>21</sup>F. Riehle et al., Metrologia **55**, 188–200 (2018).

### 3.1.2. Measurement methods

In my work, I use measurement techniques where a gas sample is placed in an optical cavity. It is both the well-known cavity ring-down spectroscopy (CRDS)<sup>22</sup> technique as well as a recently developed technique based on the measurement of optical cavity dispersive resonance mode shifts - cavity mode-dispersion spectroscopy (CMDS)<sup>23</sup> [23].

The main element of the CRDS type spectrometer is an optical cavity made of high-reflectivity mirrors (typically  $R \ge 0.9997$ ). In a typical arrangement, the cavity is pumped with a laser beam at a frequency matching the frequency of one of the cavity resonances. Thereafter, pumping is interrupted, for example by rapid frequency tuning or by switching off the pumping beam. If the pumping beam is spectrally narrow so that only one cavity resonance mode is pumped, an exponential decay in the intensity of the light leaking through one of the mirrors is recorded. Then the absorption coefficient  $\alpha$  can be determined based on the decay constant  $\tau$  from the following relationship:

$$\frac{1}{c\tau} = \alpha + \alpha_{\rm bg},\tag{1}$$

where c is the speed of light and  $\alpha_{bg}$  is the loss in the absence of absorption due to the mirrors' reflectivity and light scattering. The length of the optical path on which the beam is absorbed can reach many kilometers, which results in the very high sensitivity of CRDS spectrometers. They enable measurements of spectral lines with intensities slightly exceeding  $10^{-31}$  cm/molecule<sup>24</sup>. Their advantage is, in particular, the insensitivity to fluctuations in the power of the laser beam and the lack of the need to know the actual length of the absorption path. On the other hand, the basic limitations result from the necessity to precisely determine the time decay constants, which in typical systems range from a few to several hundred microseconds, and decrease with increasing absorption. Their determination requires fast, highly linear optical detectors and analog-to-digital converters.

An alternative to the determination of the time decay constants can be measurement of the width of the cavity mode that leads to the CMWS technique (cavity mode-width spectroscopy)<sup>25</sup>. The shape of the optical cavity mode can be described by a Lorentzian profile within a good approximation. While in the CRDS technique, with the increase of absorption, the time decay constant decreases, in the CMWS technique the width of the cavity mode increases with the increase of absorption. As a result, the CMWS technique enables accurate measurements in conditions where the time decay constant is too short and the CRDS technique no longer gives accurate results [23]. This technique does not require the use of a high-speed detector and analog-to-digital converter, however they must have a linear response.

The CMDS technique is a complementary measurement method to CRDS and CMWS. In contrast to the absorption techniques such as CRDS and CMWS, in this case the resonance dispersion in the sample is determined, which is related to the absorption by the Kramers-Krönig equations. Practically, the measurement comes down to determining the frequency shift of the cavity mode on effect of dispersion, compared to the situation of no resonant dispersion. Also in this technique, the use of fast detectors and transducers is not required. Both the vertical and the horizontal axis of the spectrum are marked with the frequency, i.e. the physical quantity that can presently be measured the most accurately<sup>26</sup>, which ensures the linearity of this measurement technique. This results in a further extension of the dynamic range compared to the CMWS technique. It is worth noting that the absorption and dispersion spectrum in the CMWS and CMDS techniques can be obtained from the same measurement, in which, based on the measurement of the shape of the cavity mode, its width or central frequency is determined. CMDS is a measurement method more accurate than CRDS and CMWS [23], while the measurement time using CMDS and CMWS methods is significantly longer than in the case of CRDS. Moreover, the CMDS technique requires tightly binding the frequency of the laser beam to the resonant mode of the cavity. Currently, it is not widely used, also due to the limited access to widely tunable electro-optical modulators, which limits the spectral range in which it can be implemented.

The above information applies to the measurement of absorption or dispersion. An important issue is also measuring the frequency of the probe beam, i.e. determining the horizontal axis of the spectrum. When high

<sup>&</sup>lt;sup>22</sup>A. O'Keefe and D. A. G. Deacon, Review of Scientific Instruments **59**, 2544–2551 (1988).

<sup>&</sup>lt;sup>23</sup>A. Cygan et al., Optics Express **23**, 14472–14486 (2015).

<sup>&</sup>lt;sup>24</sup>S. Kassi et al., Chemical Physics Letters **582**, 6–9 (2013).

<sup>&</sup>lt;sup>25</sup>A. Cygan et al., Optics Express **21**, 29744–29754 (2013), D. A. Long et al., Applied Physics B: Lasers and Optics **114**, 489–495 (2014).

<sup>&</sup>lt;sup>26</sup>T. W. Hänsch, Reviews of Modern Physics **78**, 1297–1309 (2006).

accuracy is required, measuring the probe beam frequency with a commercial wavemeter based on the Michelson interferometer is usually insufficient, as such devices are characterized by measurement uncertainty of several dozen megahertz. In the techniques described above, the relative frequency axis can be relatively simply and accurately determined based on a measurement of the cavity free spectral range (FSR), which can be done with a wavemeter, and its accuracy can be many times better than the accuracy of the wavemeter itself<sup>27</sup>. This relative frequency axis makes it possible to obtain a good quality spectra with the CRDS technique, as long as the length of the spectrometer resonance cavity is stabilized, leading to the FS-CRDS technique (frequency-stabilized cavity ring-down spectroscopy)<sup>28</sup>. In contrast, in the CMWS and CMDS techniques, as well as in dual-beam CRDS spectrometers, it is possible to more accurately determine the relative frequency by measuring the FSR based on the detuning between the lock and probe beams, which are detuned from each other by the total number of longitudinal modes of the cavity. Accurate measurement of the absolute frequency comb (OFC). This is how the probe beam frequency has been determined in most of the measurements performed with the above techniques at the Institute of Physics, NCU since 2012<sup>29</sup>. It enables both accurate measurements of the positions of the spectral lines and of the collisional line shift coefficients.

### 3.1.3. Data analysis: spectral line shapes

In the simplest approach, the shape of molecular lines in conditions where both Doppler broadening and collisional effects are significant is described by the commonly known and used Voigt profile (VP). It is a convolution of Gaussian and Lorentzian profiles, and takes into account the effects of Doppler broadening as well as collisional broadening and shifting. However, this is a simplified approach that ignores a number of effects affecting the shape of the spectral lines. There are many experimental studies showing that the use of the Voigt profile may lead to significant systematic errors<sup>30</sup>.

The line profile currently recommended by IUPAC<sup>31</sup> (International Union of Pure and Applied Chemistry) for spectral molecular databases such as HITRAN<sup>32</sup> is the Hartmann-Tran profile (HTP)<sup>33</sup>. In addition to the effects included in the VP, it takes into account a number of other, subtle effects that affect the shape of the spectral lines. The HTP takes into account the effects of the dependence of the collisional broadening and shifting on the velocity of the absorber<sup>34</sup>, which cause a narrowing of the line and its asymmetry. HTP also takes into account the effects related to the change in the absorber velocity due to collisions leading to the so-called Dicke narrowing<sup>35</sup>. In the HTP profile, these collisions are treated according to the hard collision model. In addition, HTP takes into account the correlation between phase and velocity changing collisions. The asymmetry associated with the line-mixing effect<sup>36</sup> is not included in the original HTP profile, but can be easily incorporated into it. The HTP is based on the more general expressions given by Pine<sup>37</sup>. It has been shown to be sufficiently accurate for atmospheric applications<sup>38</sup> with relatively low numerical complexity, which enables its broad application.

HTP can be simplified to obtain other commonly used line profiles. For this purpose, it is necessary to set to zero value appropriate parameters. Zeroing the correlation parameter leads to a speed-dependent Nelkin-Ghatak profile (SDNGP)<sup>39</sup>. If the parameter describing the Dicke narrowing is additionally set to zero, one gets the speed-dependent Voigt profile (SDVP)<sup>40</sup>. Moreover, zeroing the parameters describing the dependence of the

<sup>&</sup>lt;sup>27</sup>J. T. Hodges et al., Review of Scientific Instruments **75**, 849–863 (2004).

<sup>&</sup>lt;sup>28</sup>J. T. Hodges and D. Lisak, Applied Physics B: Lasers and Optics **85**, 375–382 (2006).

<sup>&</sup>lt;sup>29</sup>J. Domysławska et al., Journal of Chemical Physics **136**, 024201 (2012).

<sup>&</sup>lt;sup>30</sup>P. Duggan et al., Journal of Molecular Spectroscopy **186**, 90–98 (1997).

<sup>&</sup>lt;sup>31</sup>J. Tennyson et al., Pure and Applied Chemistry 86, 1931–1943 (2014).

<sup>&</sup>lt;sup>32</sup>I. Gordon et al., Journal of Quantitative Spectroscopy and Radiative Transfer **277**, 107949 (2022).

<sup>&</sup>lt;sup>33</sup>N. Ngo et al., Journal of Quantitative Spectroscopy and Radiative Transfer **129**, 89–100 (2013), N. Ngo et al., Journal of Quantitative Spectroscopy and Radiative Transfer **134**, 105 (2014).

<sup>&</sup>lt;sup>34</sup>P. R. Berman, Journal of Quantitative Spectroscopy and Radiative Transfer **12**, 1331–1342 (1972).

<sup>&</sup>lt;sup>35</sup>R. H. Dicke, Physical Review **89**, 472–473 (1953).

<sup>&</sup>lt;sup>36</sup>A. Pine and R. Ciurylo, Journal of Molecular Spectroscopy **208**, 180–187 (2001).

<sup>&</sup>lt;sup>37</sup>A. Pine, Journal of Quantitative Spectroscopy and Radiative Transfer **62**, 397–423 (1999), B. Lance et al., Journal of Molecular Spectroscopy **185**, 262–271 (1997).

<sup>&</sup>lt;sup>38</sup>N. Ngo et al., Journal of Quantitative Spectroscopy and Radiative Transfer **203**, 325–333 (2017).

<sup>&</sup>lt;sup>39</sup>B. Lance et al., Journal of Molecular Spectroscopy **185**, 262–271 (1997).

<sup>&</sup>lt;sup>40</sup>P. R. Berman, Journal of Quantitative Spectroscopy and Radiative Transfer **12**, 1331–1342 (1972).

collisional broadening and shifting on the absorber speed leads to the Voigt profile in its basic form. HTP can also be simplified to the Nelkin-Ghatak profile (NGP)<sup>41</sup> if the speed dependency and correlation parameters are zeroed. On the other hand, as a result of the HTP simplification, it is not possible to obtain profiles in which the velocity-changing collisions are described within the soft collision model, i.e. the Galatry profile (GP)<sup>42</sup> and its version taking into account the speed-dependence of the line broadening and shifting, i.e. speed-dependent Galatry profile (SDGP)<sup>43</sup>. Moreover, in the HTP and the profiles to which it can be simplified, the dependence of the collisional broadening and shifting on the absorber velocity is taken into account in accordance with the so-called quadratic approximation<sup>44</sup>. The second commonly used description of these effects is based on the use of confluent hypergeometric functions<sup>45</sup> and results from the assumption that the interaction potential between the absorber and perturber is of the form  $r^{-q}$ , where r is the distance between the interacting molecules.

VP is a simple profile with a relatively small number of fitted parameters, while each subsequent effect taken into account in the profile increases the number of parameters. There are nine of them in HTP: position and intensity of the line, collisional broadening and shifting, Doppler broadening, frequency of optical collisions (Dicke narrowing), two parameters related to the effects of speed-dependence of collisional broadening and shifting, and a parameter describing correlations between collisions of various types. The Doppler broadening in many cases can be determined from the temperature, but the remaining parameters are usually fitted. Typically, parameters describing the spectrum baseline are also fitted and are characterized by high uncertainty. Such a large number of fitted parameters can lead to numerical correlations between them. The influence of these correlations on the obtained line shape parameters can be reduced by using the data analysis technique, in which the spectra obtained for different pressures are analyzed simultaneously, while the individual parameters of the line shape are fitted as pressure coefficients or pressure independent values<sup>46</sup>. This fitting method is called the *multispectrum fit* technique<sup>47</sup>.

### **3.2.** Overview of the achievement: "Precise spectroscopy of weak lines of molecules of atmospheric importance"

My most important scientific achievement, entitled "Precise spectroscopy of weak lines of molecules of atmospheric importance", consists of the following series of five publications:

- H1. O. L. Polyansky, **K. Bielska**, M. Ghysels, L. Lodi, N. F. Zobov, J. T. Hodges, J. Tennyson, *High-accuracy* CO<sub>2</sub> line intensities determined from theory and experiment, Phys. Rev. Lett. **114**, 243001 (2015)
- H2. K. Bielska, S. Wójtewicz, P. Morzyński, P. Ablewski, A. Cygan, M. Bober, J. Domysławska, M. Zawada, R. Ciuryło, P. Masłowski, D. Lisak, *Absolute frequency determination of molecular transition in the Doppler regime at kHz level of accuracy*, J. Quant. Spectrosc. Radiat. T 201, 156-160 (2017)
- H3. K. Bielska, J. Domysławska, S. Wójtewicz, A. Balashov, M. Słowiński, M. Piwiński, A. Cygan, R. Ciuryło, D. Lisak, Simultaneous observation of speed dependence and Dicke narrowing for self-perturbed P-branch lines of O<sub>2</sub> B band, J. Quant. Spectrosc. Radiat. T 276, 107927 (2021)
- H4. K. Bielska, A. Cygan, M. Konefał, G. Kowzan, M. Zaborowski, D. Charczun, S. Wójtewicz, P. Wcisło, P. Masłowski, R. Ciuryło, D.Lisak, *Frequency-based dispersion Lamb-dip spectroscopy in a high finesse optical cavity*, Opt. Express 29, 39449-39460 (2021)
- H5. K. Bielska, A. A. Kyuberis, Z. D. Reed, G. Li, A. Cygan, R. Ciuryło, E. M. Adkins, L. Lodi, N. F. Zobov, V. Ebert, D. Lisak, J. T. Hodges, J. Tennyson, O. L. Polyansky, *Subpromille measurements and calculations* of CO (3–0) overtone line intensities, Phys. Rev. Lett. **129**, 043002 (2022)

<sup>&</sup>lt;sup>41</sup>M. Nelkin and A. Ghatak, Physical Review **135**, A4–A9 (1964).

<sup>&</sup>lt;sup>42</sup>L. Galatry, Physical Review **122**, 1218–1223 (1961).

<sup>&</sup>lt;sup>43</sup>R. Ciurylo and J. Szudy, Journal of Quantitative Spectroscopy and Radiative Transfer **57**, 411–423 (1997).

<sup>&</sup>lt;sup>44</sup>D. Priem et al., Journal of Molecular Structure **517-518**, 435–454 (2000).

<sup>&</sup>lt;sup>45</sup>J. Ward et al., Journal of Quantitative Spectroscopy and Radiative Transfer **14**, 555–590 (1974).

<sup>&</sup>lt;sup>46</sup>A. Pine and R. Ciurylo, Journal of Molecular Spectroscopy **208**, 180–187 (2001), A. Pine and T. Gabard, Journal of Quantitative Spectroscopy and Radiative Transfer **66**, 69–92 (2000).

<sup>&</sup>lt;sup>47</sup>D. C. Benner et al., Journal of Quantitative Spectroscopy and Radiative Transfer **53**, 705–721 (1995).

Among them, the work [H4], published in the *Optics Express* journal, was featured as "Editor's pick", while the work [H5], published in the *Physical Review Letters* journal, was awarded the "Editors' Suggestion" distinction.

### 3.2.1. Line intensities: carbon dioxide

The basic model of the molecule spectrum contains information on the positions and intensities of the spectral lines, disregarding the other parameters of the line shape. It turns out, however, that even at such a basic level, we encounter significant difficulties, in particular in terms of determining the line intensities with the expected promille accuracy. Data obtained with experimental methods by different research teams are often inconsistent with each other. When several experimental results are available for a given line, the relative differences between them are often of several percent. A good example is the spectrum of carbon monoxide. The available experimental results for its individual bands can be found in the recent work of Meshkov et al.<sup>48</sup>, where in the (3 - 0) band measured by many experimental groups, the differences between individual results often exceed 2%, and sometimes as much as 5%. Likewise, theoretical results are often inconsistent with the experimental ones.

Measurement methods characterized by the highest accuracy are usually time-consuming and practically it is possible to perform measurements with high accuracy only for a limited number of spectral lines. Fourier transform spectroscopy is a measurement technique that enables broadband measurements. However, significant difficulties in this technique are related to the proper consideration of the apparatus function and the determination of the exact absorption pathlength, which is one of the reasons for the discrepancies between the literature data.

On the other hand, from the theoretical point of view, the level of complication of even relatively small molecules, such as carbon monoxide or carbon dioxide, definitely exceeds the current capabilities of calculating line intensities with the *ab initio* methods. Theoretical calculations of the line intensity require the determination of the dipole moment surface (DMS) and the potential energy surface (PES). Currently, effective *ab initio* calculations of the DMS are possible<sup>49</sup>, while in the case of PES, better results than from purely *ab initio* calculations arise from the use of semi-empirical ones<sup>50</sup>.

The work [H1] shows the high efficiency of such a method: a group from University College London (UCL) performed calculations of the carbon dioxide line intensities, which were based on DMS calculated using the ab *initio* method and available in the literature semi-empirical PES<sup>51</sup>. The calculated line intensities were compared with the results of measurements carried out at NIST. The experimental part of the work consisted in measuring the intensities of 27 lines from the band (30013) - (00001) of the carbon dioxide molecule, located in the spectral range around 1.6  $\mu$ m. Measurements were made using the FS-CRDS technique (frequency-sabilized cavity ring-down spectroscopy), i.e. the cavity ring-down spectroscopy with active stabilization of the optical cavity length using a frequency-stabilized laser, which in this case was helium-neon laser. The difference from the most common approach to FS-CRDS spectroscopy was the use of an electro-optical modulator (EOM) to tune the beam frequency, which greatly accelerated the measurements<sup>52</sup>. The intensities of the measured lines were, as for the CRDS technique, relatively high and ranged between  $8 \times 10^{-25}$  cm/molecule and  $2 \times 10^{-23}$  cm/molecule. For this reason, a sample of carbon dioxide in air was used in the measurements. The optical cavity construction was made of electro-polished stainless steel. Nevertheless, carbon dioxide adsorption and desorption effects on the cavity walls were observed. To avoid the associated variation of the carbon dioxide content in the sample, measurements were made under gas flow conditions through the cavity. The simulations of the influence of etalons present in the measurement system on the determined line intensities were also performed. The experimentally determined line intensities were characterized by relative standard uncertainties between 0.1% and 1%, whereas for most of the lines they did not exceed 0.2%.

The mean, relative difference between the theoretical and experimental results presented in the paper was 0.33%, with a standard uncertainty of 0.05%. This is the first time that such a good agreement has been achieved between the measured and theoretically predicted intensities of molecular lines. This compliance meets the

<sup>49</sup>L. Lodi et al., Journal of Chemical Physics **135**, 034113 (2011).

<sup>&</sup>lt;sup>48</sup>V. V. Meshkov et al., Journal of Quantitative Spectroscopy and Radiative Transfer **280**, 108090 (2022).

<sup>&</sup>lt;sup>50</sup>E. Zak et al., Journal of Quantitative Spectroscopy and Radiative Transfer **177**, 31–42 (2016), I. I. Mizus et al., Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences **376**, 20170149 (2018).

<sup>&</sup>lt;sup>51</sup>X. Huang et al., The Journal of Chemical Physics **136**, 124311 (2012).

<sup>&</sup>lt;sup>52</sup>G.-W. Truong et al., Nature Photonics **7**, 532–534 (2013).

requirements for the data used to interpret remote atmospheric measurements. It was the first such dataset for carbon dioxide, as the reference data used at that time was characterized mostly by relative standard uncertainties of a few percent<sup>53</sup>. Boudjaar et al.<sup>54</sup> determined the line intensities, most of which have assigned sub-percent standard uncertainties, but line intensity values are clearly higher than our theoretical and experimental results. On the other hand, the data available in the literature of the declared sub-percent standard uncertainties for the band (20012) – (00001) were not consistent with each other<sup>55</sup> and except for the intensity of one line determined by Wübbeler et al.<sup>56</sup> were not consistent with our theoretical results. However, more important than obtaining such a good agreement of theory and experimental data of high accuracy, allows to effectively predict the line intensities. The results obtained for other bands were later confirmed by Odintsova et al.<sup>57</sup>, where the intensities of three lines from the carbon dioxide band (20012) – (00001) again at a sub-percent level agreed with the results of the calculations.

### 3.2.2. Measuring the position of the Doppler-broadened line with kilohertz level accuracy

In the work [H2] the position of the Doppler-broadened line from the B band of molecular oxygen (line P7 P7) was determined with reference to the atomic frequency standards: the strontium optical atomic clock (<sup>88</sup>Sr) of a short time (1 s) relative stability of the optical frequency of  $4.3 \times 10^{-14}$  and hydrogen maser (short-term relative stability  $10^{-12}$ ). Their long-term relative stabilities are below  $10^{-16}$  and below  $10^{-15}$ , respectively. This work demonstrates a proof-of-principle experiment in which the optical atomic clock was used for the first time as the optical frequency reference in molecular spectroscopy. The CRDS spectrometer was linked with the optical clock via an optical frequency comb by simultaneously beating with the comb both the spectrometer probe beam and the optical atomic clock beam. In this system, the frequency difference between the spectrometer probe beam and the clock beam was determined with an optical frequency comb, for which the reference frequency was the RF signal from the hydrogen maser sent via optical fiber<sup>58</sup>.

The central frequency of the investigated line was determined with a standard uncertainty of 8.2 kHz, which corresponds to a relative standard uncertainty of  $2 \times 10^{-11}$ . Such accuracies are typically obtained by a Doppler-free techniques (e.g. saturation spectroscopy). Also, the collisional shift coefficient was determined with sub-percent accuracy (relative standard uncertainty  $7 \times 10^{-3}$ ). The main limitation of the measurement precision was the stability of the optical cavity, not of the reference frequencies. The paper shows that using only the signal from the hydrogen maser, without the use of an optical clock, would lead to results two orders of magnitude less precise, if there were no constraints due to the stability of the optical cavity.

Obtaining such small uncertainty of the line position was possible thanks to the use of a stable frequency standard and long-term averaging of the spectra. The result of these works was the construction of a new version of the spectrometer. Its operation has been fully demonstrated in [H3].

Saturation measurements, which seem a natural and simpler way to obtain line positions with comparable accuracy, in molecular spectroscopy are successfully performed for spectral lines of higher intensities. However, the B-band spectral lines of oxygen are relatively weak. They result from magnetic-dipole transitions, not electric-dipole ones, and have intensities below  $6 \times 10^{-25}$  cm/molecule. Lines of this kind have not been measured by saturation spectroscopy methods so far, because their saturation requires a high power of the pumping beam. The first attempts to carry out saturation measurements in the B band of oxygen were recently made in the Institute of Physics of the Nicolaus Copernicus University in Toruń with my participation. They resulted with line positions characterized by standard uncertainties of values between 10 kHz and 20 kHz, so at present they are not competitive with the measurements carried out for the Doppler-broadened line presented in this paper.

<sup>&</sup>lt;sup>53</sup>K. Song et al., Journal of Quantitative Spectroscopy and Radiative Transfer **111**, 332–344 (2010), B. Perevalov et al., Journal of Molecular Spectroscopy **252**, 190–197 (2008), L. Wang et al., Journal of Molecular Spectroscopy **234**, 84–92 (2005).

<sup>&</sup>lt;sup>54</sup>D. Boudjaadar et al., Journal of Molecular Spectroscopy, 158–167.

<sup>&</sup>lt;sup>55</sup>G. Wübbeler et al., The Journal of Chemical Physics **135**, 204304 (2011), G. Casa et al., The Journal of Chemical Physics **127**, 084311 (2007), G. Casa et al., Journal of Chemical Physics **130**, 184306 (2009).

<sup>&</sup>lt;sup>56</sup>G. Wübbeler et al., The Journal of Chemical Physics **135**, 204304 (2011).

<sup>&</sup>lt;sup>57</sup>T. A. Odintsova et al., The Journal of Chemical Physics **146**, 244309 (2017).

<sup>&</sup>lt;sup>58</sup>P. Morzyński et al., Scientific Reports **5**, 17495 (2015).

### 3.2.3. Simultaneous observation of speed-dependence and Dicke narrowing in the oxygen B band

After performing the measurements presented in [H2], the spectrometer was significantly reconfigured. The laser used to stabilize the optical cavity length of the spectrometer has been replaced. The probe and lock beams were separated, which made it possible to obtain an experimental setup similar to that described in the work of Cygan et al.<sup>59</sup>. As a result of the research carried out with my participation and described in the paper [22], the electronical system used to switch off the beam during the registration of ring-down decays has been rebuilt. This way, the extinction ratio was increased, i.e. the ratio of the power of the probe beam pumping the optical cavity to the residual power present in the system after it was turned off, which improved the accuracy of the determined time decay constants [22]. A system for active stabilization of the cavity temperature was also built. The new version of the spectrometer was used in some of the measurements presented in [24], but its capabilities were fully exploited for the first time in [H3].

The work [H3] presents the results of measurements of the shape of self-perturbed spectral lines from the oxygen B band, in the low pressure range: up to 22 Torr (2.9 kPa) in the case of the P1 P1 line and below 10 Torr (1.3 kPa) for lines P7 P7 and P9 P9. In previous works on the shape of the oxygen B-band lines, in the low pressure range, the profile describing the line shape to a sufficient degree was SDVP [20]. In the paper [H3] the signal to noise ratio was up to eight times higher compared to previous measurements of the same lines from the P branch<sup>60</sup>. The shapes of the measured lines obtained in this way cannot be described using the SDVP profile. The simplest profile that reflects the shape of these lines well enough is SDNGP. This means that speed-dependent effects and the Dicke narrowing were observed simultaneously.

A detailed analysis of the systematic uncertainty of the line shape parameters was performed. In particular, in addition to CRDS measurements, CMWS measurements were also carried out. The signal to noise ratio of the spectra obtained with the CMWS technique is significantly lower, however, they were used to estimate the uncertainty of the obtained line shape parameters. Using the results obtained with the CMWS technique, it was also shown that the uncertainty introduced by the possible non-linearity of the detection system in the CRDS technique is insignificant compared to the other sources of uncertainty. This conclusion was based on simulations that took into account two different detection system nonlinearity models. The simulations showed that for both probable types of nonlinearity, the measurements with the CRDS and CMWS techniques should lead to a line intensity with a systematic error of the opposite sign. Hence, based on the comparison of the obtained line intensities, it was found that the impact of any non-linearity on the results was insignificant. This conclusion is particularly important from the point of view of the CRDS technique, which is based on the precise determination of very short decay constants (in the presented system  $\tau \leq 13 \ \mu s$ ). It has been shown that after introducing into the spectrometer the changes presented above, it is possible to determine the line positions with standard uncertainties in the range between 20 kHz and 30 kHz without long-term averaging of the spectra, which was needed in the work [H2]. In addition, systematic differences from the results of previous measurements of line intensities in the oxygen B-band obtained in our laboratory were observed, which probably results from previous leaks in the gas supply system. The line intensities were obtained with relative standard uncertainties of 0.2%.

In this work, the effect of changing the cavity mirrors reflectivity due to illumination with a beam of relatively high power was also observed, which can be related to the light absorption in the mirrors. The paper shows that with the appropriate choice of measurement conditions, the obtained results are not burdened with additional uncertainty related to the light absorption by the mirrors.

### 3.2.4. Saturation spectroscopy: determination of line positions with sub-kilohertz accuracy

In the work [H2] the position of the Doppler-broadened spectral line was determined with a standard uncertainty of several kHz. The next step in increasing the accuracy is the transition to measurements using Doppler-free spectroscopy methods. The work [H4], which was featured as the "Editor's pick", presents a new method of dispersion measurements in saturation regime, i.e. measurements of the so-called Lamb dips. It is the first implementation of saturation measurements using the CMDS technique. In this work, the CMWS technique was also used for the first time in saturation measurements, as well as the CRDS technique, which has already been used many times in saturation measurements in the optical cavity.

<sup>&</sup>lt;sup>59</sup>A. Cygan et al., Journal of Chemical Physics **144**, 214202 (2016).

<sup>&</sup>lt;sup>60</sup>S. Wójtewicz et al., Journal of Quantitative Spectroscopy and Radiative Transfer 144, 36–48 (2014).

It has been shown that, contrary to expectations, the CRDS technique used for measurements under saturation conditions may lead to inaccurate results. This is due to its sensitivity to fluctuations of the saturating beam power. A similar issue was observed in the case of CMWS measurements, where the results turned out to be even less accurate. On the other hand, the results obtained with the CMDS technique were characterized by the highest accuracy, similarly to the measurements of Doppler-broadened lines [23]. Also similarly to Doppler measurements, the CMDS technique offers the greatest dynamic range among the three considered techniques. The advantage of the CMDS technique over the CRDS and CMWS techniques results from the insensitivity of the dispersion Doppler-broadened profile envelope to the saturation effect in the case when the homogeneous line width is very small compared to the Doppler width<sup>61</sup>. On the other hand, in absorption techniques (e.g. CRDS, CMWS), the change in the power of the pumping beam leads to the asymmetry of the Doppler envelope and thus the recorded Lamb dip. This results in a change of its determined position, which is not the case in dispersion measurements using the CMDS technique.

Measurements were made for two lines from the (3 - 0) carbon monoxide band. They led to line positions with standard uncertainties below 0.5 kHz, which is presently the most accurate result for these lines. The work contributes to the discussion on the pressure shift of the line measured under saturation conditions. In the work of Wang et al.<sup>62</sup>, in which one of the lines considered in [H4] was also measured with the saturation method, no pressure shift was observed. On the other hand, there are studies showing that, unlike measurements of Doppler-broadened lines under relatively high pressures where the line shift is linear with pressure, under saturation conditions this relation may be non-linear<sup>63</sup>. Moreover, a common approach in determining undisturbed line position in saturation measurements is to measure it at only one pressure and then to determine the undisturbed position of the line, based on its pressure shift coefficient derived for Doppler-broadened line<sup>64</sup>. In the pressure range studied in [H4], under saturation conditions, a clear pressure shift of the line under saturation conditions was observed. At the same time, no clear deviations from the linear dependence of the line position on the pressure were observed, and the determined value of the pressure shift coefficient is lower by about 40% than the literature values from Doppler measurements<sup>65</sup>, however, the relative standard uncertainty of these results is close to 30%.

### 3.2.5. Promille accuracy of the line intensity determination: carbon monoxide

In the already mentioned work [23] it was shown that the CMDS technique enables much more accurate measurements of spectral line intensities than the CRDS technique in its standard implementations. The results presented in the study suggested that it is possible to obtain promille accuracy. In order to confirm such a good accuracy of the measurements, the studies presented in the paper [H5], which was featured as "Editors' Suggestion", were performed. For this purpose, cooperation was established with the leading optical metrology groups from the National Institute of Standards and Technology (NIST, USA) and Physikalisch-Technische Bundesanstalt (PTB, Germany) and a group of theoreticians from UCL, dealing with calculations of the line intensities. As the experimental object, we chose a carbon monoxide molecule, which is one of the key molecules for the study of the atmosphere.

A group of theoreticians from UCL carried out calculations of line intensities for the  ${}^{12}C^{16}O$  molecule. The carbon monoxide molecule has a simpler structure than the carbon dioxide molecule studied in [H1], hence more accurate calculations are possible. The dipole moment surfaces ere determined in the *ab initio* calculations, while the potential energy surfaces were semiempirical<sup>66</sup>.

As with the calculation, the carbon monoxide molecule is a good experimental object. Accurate measurements are easier than in the case of a carbon dioxide due to the less complicated structure of the spectrum and the smaller number of blending lines, and coming from other isotopologues. Moreover, in the case of carbon monoxide, the adsorption and desorption on the surface of the stainless steel absorption cell is at a level undetectable in our experimental configuration, while in the case of carbon dioxide (work [H1]) it was a significant limitation.

The experimental part of the work was performed independently in three laboratories, and concerned the

<sup>&</sup>lt;sup>61</sup>W. Ma et al., Journal of the Optical Society of America B 25, 1144–1155 (2008).

<sup>&</sup>lt;sup>62</sup>J. Wang et al., Journal of Chemical Physics 147, 091103 (2017).

<sup>&</sup>lt;sup>63</sup>S. N. Bagaev and V. P. Chebotaev, Soviet Physics Uspekhi **29**, 82–103 (1986).

<sup>&</sup>lt;sup>64</sup>J. Burkart et al., Journal of Chemical Physics **142**, 191103 (2015).

<sup>&</sup>lt;sup>65</sup>N. Picqué and G. Guelachvili, Journal of Molecular Spectroscopy 185, 244–248 (1997).

<sup>&</sup>lt;sup>66</sup>J. A. Coxon and P. G. Hajigeorgiou, The Journal of Chemical Physics 121, 2992–3008 (2004).

measurements of the line intensities from the carbon monoxide band (3 - 0). Relatively strong lines were measured with Fourier transform spectroscopy (FTS) technique in PTB<sup>67</sup>. In addition, seven weaker lines were selected and were independently measured in two laboratories: at the Institute of Physics of the Nicolaus Copernicus University using the CMDS method, and at NIST using the CRDS technique with a calibrated analog-to-digital converter to reduce the non-linearity of the detection system<sup>68</sup>. For all measurements, the relative standard uncertainties of the line intensities do not exceed 2‰, and in some cases are less than 1‰. The relative differences between the intensities determined in the measurements carried out at NCU and NIST are about 1‰, only for the weakest measured line, P30, the difference is greater. For the first time, such a good agreement of the line intensity measurements from different laboratories and performed with significantly different techniques: absorption and dispersion, was obtained.

All measurement results were compared with the results of theoretical calculations. The mean relative difference between the experimental and theoretical line intensities is 0.6‰ and its standard uncertainty is 0.9‰. It is the first time that such a good agreement is obtained between the experimental and theoretical values of the molecular line intensities. The use of various measurement techniques, characterized by optimal performance for lines with significantly different intensities, allowed for comparison with the theory of line intensities from a wide range of values, which corresponds to a wide range of rotational energies in the lower state. Comparison with the theory allows to indirectly state that the measurements made with the FTS technique are also consistent at the promille level with the measurements made in other laboratories. Also in this case, it is unprecedented in the literature. The paper shows that the compliance of these measurements with the theoretical results is more than an order of magnitude better than in the case of the data available in the literature for the band (3 - 0). A comparison with data available in the widely used HITRAN<sup>69</sup> database is also shown. It has been shown that while the new results are consistent with the HITRAN database for relatively high values of the J quantum number in the R branch, for low values and in the P branch, differences significantly exceeding 1% are observed. Similarly, there is a significant difference between the present theoretical results and the latest literature values for this band, which are based on semi-empirical calculations using available experimental data for five different carbon monoxide absorption bands<sup>70</sup>.

### 3.2.6. Summary of the achievement

To sum up, my research work led to obtaining precise and accurate values of the line shape parameters. These are mainly the intensities and positions of the lines, as well as the collisional parameters necessary for the correct spectra simulation. The achievement consists in particular of:

- 1. Development of experimental systems and measurement techniques leading to the reduction of systematic uncertainties. I proposed a new dispersion measurement method in saturation spectroscopy and showed that it leads to more accurate results than the commonly used absorption technique.
- 2. Demonstration that the technique of dispersion measurements enables measurements of the line intensity with promille relative standard uncertainties, and under the conditions of saturation spectroscopy the line positions with sub-kilohertz accuracy.
- 3. Collaboration with the theoretical group to obtain parameters, here line intensities, in a wide spectral range, including lines and bands outside the experimental range. For the first time, the results of line intensity measurements, made with different techniques in different laboratories, agree with each other and with the theoretical results at the promille and subpromille levels, i.e. an order of magnitude better than most of data available in the literature.
- 4. Accurate, even at the sub-kilohertz level, determination of the line positions in order to provide data that can be used in the study of basic concepts.
- 5. Determination of accurate line shape parameters needed in the most demanding remote observations of the Earth's atmosphere, with particular emphasis on line intensities, along with the determination of

<sup>&</sup>lt;sup>67</sup>V. Werwein et al., Applied Optics **56**, E99 (2017).

<sup>&</sup>lt;sup>68</sup>A. J. Fleisher et al., Physical Review Letters **123**, 043001 (2019).

<sup>&</sup>lt;sup>69</sup>I. Gordon et al., Journal of Quantitative Spectroscopy and Radiative Transfer **277**, 107949 (2022).

<sup>&</sup>lt;sup>70</sup>V. V. Meshkov et al., Journal of Quantitative Spectroscopy and Radiative Transfer **280**, 108090 (2022).

systematic contributions to the uncertainty of individual parameters. In particular, the influence of the non-linearity of the detection system in the CRDS type spectrometer, which is often ignored in such estimations, was accounted for.

6. Introduction of an optical atomic clock as a frequency reference for measuring positions of spectral lines into the molecular spectroscopy.

### **3.3.** Other achievements

### 3.3.1. Ice vapor pressure

In the paper [9], a new method of measuring the dependence of saturated vapor pressure of ice on temperature was proposed. A water vapor generator, i.e. an ice-covered saturator, which was used to calibrate hygrometers at NIST (NIST Primary Standard Humidity Generator) was connected to the FS-CRDS spectrometer. Its temperature was uniform, stable, and known within millikelvin accuracy. This saturator was the source of the sample, which was gaseous nitrogen saturated with water vapor at a temperature corresponding to the temperature of ice. Then, the absorption corresponding to the certain spectral line of water vapor was measured with the FS-CRDS spectrometer. These lines were selected depending on the water vapor content in the sample to obtain absorption values optimal for the spectrometer, leading to the highest measurement accuracy. The knowledge of the approximate absolute values of the water vapor pressure. An important advantage of this approach is that the measurement accuracy is independent on the accuracy of the assumed line intensities. Only relative line intensities determined in these measurements were important. The measurements were made in reference to the accurately known value of the saturated vapor pressure of the ice at the water triple point<sup>71</sup>. This value is known with a relative standard uncertainty of  $5 \times 10^{-6}$ .

Earlier studies on the dependence of the saturated ice vapor pressure on temperature were carried out using various techniques. In the literature one can find both experimental data and analytical expressions obtained on the basis of the analysis of experimental data or thermodynamic calculations. These calculations differ mainly in the assumptions regarding the dependence of the sublimation heat on the temperature and the treatment of water vapor as an ideal gas or taking into account the appropriate corrections allowing the use of a gas model closer to the real one. Comparison of the literature data showed that the scatter of the experimental data is an order of magnitude larger than the differences between the theoretical curves. In particular, the available experimental data did not allow, due to the low accuracy, to verify the thermodynamic calculations.

The paper [11] presents the results of measurements of the dependence of the saturated vapor pressure of ice on the temperature for temperatures ranging from 175 K to 253 K, carried out with the above-described method. They are characterized by sub-percent standard uncertainties (below 0.5% in most of the measurement temperature range). This is the first set of experimental data that allowed the verification of commonly used analytical expressions describing the dependence of ice vapor pressure on temperature. In particular, the results allowed to state that the function recommended in the work of Wagner et al.<sup>72</sup> and by IAPWS (International Association for the Properties of Water and Steam)<sup>73</sup> in the temperature range below 200 K describes this dependence much more accurately than the curve recommended by WMO (World Meteorological Organization)<sup>74</sup>. The results presented in the papers [9, 11] were the basis for my doctoral dissertation.

### 3.3.2. Spectroscopic techniques development

A significant part of my work to date has been devoted to the development of spectroscopic techniques using optical cavities, in particular the CRDS technique. Apart from the elements introduced in the spectrometers used in the works [H1-H5], I participated in the construction of the first FS-CRDS type spectrometer in Poland [5], and then in the works that led to the development of its subsequent versions. In particular, I participated in the work on the PDH (Pond-Drever-Hall)<sup>75</sup> locking technique of the spectrometer probe beam to the resonance

<sup>&</sup>lt;sup>71</sup>L. A. Guildner et al., Science **191**, 1261–1261 (1976).

<sup>&</sup>lt;sup>72</sup>W. Wagner et al., Journal of Physical and Chemical Reference Data **40**, 043103 (2011).

<sup>&</sup>lt;sup>73</sup>*Revised release on the pressure along the melting and sublimation curves of ordinary water substance* (The International Association for the Properties of Water and Steam, 2008).

<sup>&</sup>lt;sup>74</sup>Guide to meteorological instruments and methods of observation (World Meteorological Organization, 2008).

<sup>&</sup>lt;sup>75</sup>R. W. P. Drever et al., Applied Physics B **31**, 97–105 (1983).

frequency of the optical cavity. The paper [6] shows that such a lock leads to a significant increase in the signal-to-noise ratio of the recorded spectra (by a factor of about 3), and thus enables more precise determination of the line shape parameters. The paper [12] presents a detailed comparison of the FS-CRDS technique with and without the PDH lock. In the work [22] this spectrometer was used in a system in which the lock beam, used to tightly lock the laser frequency to the frequency of the cavity resonance mode, and the probe beam detuning from the cavity resonance and its incomplete switching off on the determined time decay constant and thus the absorption. It has been shown that the incomplete switching off of the beam and its detuning from the resonant frequency lead to non-exponential decay of the light intensity, which may lead to a systematic error of up to 0.5% of the decay constant value and, consequently, to systematic errors in the spectra determined on its basis. The response of the optical cavity to non-resonant excitation was analyzed, which resulted in a new measurement technique<sup>76</sup>.

I participated in the works which led to the demonstration that the dispersion measurement technique, CMDS, is more accurate than the CRDS technique. The CMDS technique was proposed by Cygan et al.<sup>77</sup>. Although from the beginning it was a promising technique<sup>78</sup>, only in the work [23] it was refined and it was possible to show its advantage over the commonly used CRDS technique and also the new CMWS technique<sup>79</sup>. It has been shown that the CMDS technique is characterized by the highest accuracy among these three techniques and at the same time gives accurate results in the widest dynamic range. My role in this work was to prepare a part of the software controlling the experiment.

I participated in the presentation of the absorption measurement technique with the use of two optical frequency combs produced with the use of Mach-Zehnder modulators from a continuous wave laser [16]. In this system, the precise phase locking of the combs to the optical cavity is crucial, which was my role in this research. The advantage of this technique, compared to the use of two independent frequency combs based on femtosecond lasers, is higher optical power in a single comb tooth and control over the relative detuning of the combs without the need for a phase lock between them. The measurement system enabled the recording of a spectrum with a width of about 4 GHz in a few microseconds.

In the work [15] a new measurement technique was proposed, which utilizes the differential measurement of absorption using the CRDS technique. It allows to reduce the impact of the so-called etalons on the spectrum. These are periodic structures that appear in the spectrum background. The presence of etalons results from the existence of coupled cavities in the system, formed when a weakly reflecting surface (e.g. a lens or a detector) is parallel to the mirror of the optical cavity. Their existence causes an effective change of the measured mirrors reflectivity and thus its finesse<sup>80</sup>. It has been shown that using the differential measurement one can obtain spectra with a much higher quality of the fit (QF) value. Although it increases the noise, due to the reduction of systematic effects it is possible to average spectra efficiently. In this way, a spectrum was obtained with a signal to noise ratio, SNR  $\approx 1.7 \times 10^5$ , comparable to the highest values obtained at that time in molecular spectroscopy<sup>81</sup> by averaging approximately ten times smaller number of spectra than in the cited paper. For comparison, in the case of standard measurements using the CRDS technique, the SNR  $\approx 7 \times 10^4$  was obtained by averaging the same number of recorded spectra. This result was obtained using a two-channel measurement in which the measurement of the absorption at spectral points distant by  $\Delta \nu$  occurred directly, one after the other. The effect of improving the quality of the spectra can also be obtained by treating the spectrum measured in a standard way as differential one, which leads to a one-channel differential measurement. Then, however, the improvement is less significant which results from the different dynamics of these measurements.

#### **3.3.3.** Investigation of the impact of collisional effects on the spectral lineshapes

I participated in a number of works devoted to determining the parameters of the shape of spectral lines for molecules important for the study of the Earth's atmosphere, in particular oxygen B band. The oxygen B band is

<sup>&</sup>lt;sup>76</sup>A. Cygan et al., Communications Physics **4**, 14 (2021).

<sup>&</sup>lt;sup>77</sup>A. Cygan et al., Optics Express **23**, 14472–14486 (2015).

<sup>&</sup>lt;sup>78</sup>A. Cygan et al., Journal of Chemical Physics **144**, 214202 (2016), A. Cygan et al., Measurement Science and Technology **27**, 045501 (2016).

<sup>&</sup>lt;sup>79</sup>A. Cygan et al., Optics Express **21**, 29744–29754 (2013), D. A. Long et al., Applied Physics B: Lasers and Optics **114**, 489–495 (2014).

<sup>&</sup>lt;sup>80</sup>J. Courtois and J. T. Hodges, Optics Letters **37**, 3354 (2012).

<sup>&</sup>lt;sup>81</sup>A. Cygan et al., Physical Review A **85**, 022508 (2012).

the second band in terms of intensity in the red part of the spectrum. It is used, in addition to the A-band, in remote measurements of the Earth's atmosphere. Although it is about 15 times weaker than the A band, it can be used together with the A band to increase the accuracy of the measurements. Prior to 2010, the exact values of the line parameters in this band were unknown. In earlier experimental works, only some of their parameters were determined: only intensities and widths<sup>82</sup>, pressure shifts<sup>83</sup>, positions and intensities<sup>84</sup>, broadenings and shifts<sup>85</sup>. The HITRAN database, in the 2012 edition<sup>86</sup>, contained new data from the work of Gordon et al.<sup>87</sup>. The uncertainty of the line intensities was 5% to 10%, contrary to the accuracy expectations at sub-percent level. At the Institute of Physics of the Nicolaus Copernicus University experimental work was carried out since 2010, parallel to the development of the CRDS measurement technique, which led to the update of the knowledge on the oxygen B band. So far, the parameters of over 60 self-perturbed lines from this band have been determined. In previous experimental works, the parameters of the shape of these lines were determined from Voigt profile fits. On the other hand, in the works that were done at the Institute of Physics of the Nicolaus Copernicus University, it was systematically shown that this profile did not correctly describe the shape of the oxygen B-band lines. The simplest profile properly describing their shape in the applied measurement conditions is SDVP, while in the case of measurements with the highest signal to noise ratio (of the order of  $4 \times 10^4$ ), despite a low pressure range (about 1 kPa), such a profile is the speed-dependent Nelkin-Ghatak [H3]. Also, in the case of weak lines, measured in a relatively high pressure range, it is necessary to use the SDNGP profile [24]. I participated in most of the works on determining the oxygen line shape parameters [5, 14, 18, 20, 24], in particular including measurements in the R branch of this band. We have also recently demonstrated the existence of a particularly strong line-mixing effect in the B band [27].

I was involved in measuring the lineshape of the carbon dioxide. In the work [7] the shape of the R16 line from the (30012) - (00001) band in a mixture of gases with a composition similar to air was investigated. The simultaneous occurrence of speed-dependence and Dicke narrowing effects was shown as well as the fact that neglecting the line narrowing effects may lead to significant systematic errors: the use of the Voigt profile leads to line intensity, which may differ by up to 2% from that determined in the study [7]. The choice of the line was dictated by the demand resulting from the remote sensing, in particular the program for monitoring carbon dioxide in the atmosphere ASCENDS (Active Sensing CO<sub>2</sub> Emissions over Nights Days and Seasons)<sup>88</sup> planned by NASA at that time.

The work [13] shows the influence of the composition of the sample on the operation of commercially available instruments used to measure  $CO_2$ , the operation of which is based on the CRDS technique. The paper compares the results obtained with the use of commercial CRDS spectrometers and devices based on chromatographic methods with measurements carried out in laboratory conditions, with a full data analysis performed. It has been shown that the variable argon content in the sample causes systematic errors in the results obtained with commercial CRDS spectrometers, the operation of which is based on the measurement of maximum absorption, not the line shape as in laboratory measurements. In particular, it has been shown that the calibration of such commercial devices requires the use of argon-containing synthetic air samples and we recommended to use natural standard air samples for calibration in order to reduce systematic errors.

### 3.3.4. Optical atomic clock: ultra-stable laser

The first optical atomic clock in Poland [10, 17] was built in Toruń, and I participated in its construction. I worked on the construction of a stable, spectrally narrow laser, which is used in the optical clock system to optically cool strontium atoms. A system based on an ECDL laser was built. Two lasers with spectral widths below 200 kHz and below 1 MHz were narrowed down with the PDH technique. For this purpose, two independent, specially designed, stable optical cavities made of glass with a very low coefficient of thermal expansion (ULE, ultra-low expansion) were used. Due to the construction of a system of two narrow lasers, it was possible to determine their width based on the optical beat-note signal. Assuming equal spectral widths, each of them was approximately

<sup>&</sup>lt;sup>82</sup>L. P. Giver et al., Journal of Quantitative Spectroscopy and Radiative Transfer **14**, 793–802 (1974).

<sup>&</sup>lt;sup>83</sup>A. J. Phillips and P. A. Hamilton, Journal of Molecular Spectroscopy 174, 587–594 (1995).

<sup>&</sup>lt;sup>84</sup>S.-L. Cheah et al., Journal of Quantitative Spectroscopy and Radiative Transfer **64**, 467–482 (2000).

<sup>&</sup>lt;sup>85</sup>J. E. Barnes and P. B. Hays, Journal of Molecular Spectroscopy **216**, 98–104 (2002).

<sup>&</sup>lt;sup>86</sup>L. S. Rothman et al., Journal of Quantitative Spectroscopy and Radiative Transfer **130**, 4–50 (2013).

<sup>&</sup>lt;sup>87</sup>I. E. Gordon et al., Journal of Quantitative Spectroscopy and Radiative Transfer **112**, 2310–2322 (2011).

<sup>&</sup>lt;sup>88</sup>S. R. Kawa et al., Tellus B: Chemical and Physical Meteorology **62**, 759–769 (2010).

8.4 Hz [8]. This system was also used in a configuration where one of the lasers was PDH locked to the cavity and then the other laser was phase locked to it. This resulted in a tunable laser system capable of measuring narrow structures such as the  ${}^{1}S_{0} - {}^{3}P_{1}$  line, used in an optical clock, of a natural width below 7 kHz. This laser was also used to measure the absolute frequency of the probe laser in the CRDS spectrometer [14]. On the other hand, in paper [4], the pressure shift and broadening coefficients for this line, perturbed by noble gases, in the low pressure range were determined theoretically and experimentally. Unlike most of my publications, in this case my contribution was to determine the theoretical values of these coefficients.

The optical atomic clock, which later expanded to a system of two clocks, was used in a number of works that are beyond the atomic physics. In particular, it was used to search for dark matter. These works, carried out with the use of the clocks<sup>89</sup> and the global network of optical atomic clocks<sup>90</sup>, made it possible to reduce the estimated value of the postulated interaction constant between dark matter and known matter by orders of magnitude. The use of an optical atomic clock as a frequency standard for radio astronomy observations made in the VLBI network (Very Long Base Interferometry) was also shown<sup>91</sup>.

### 3.3.5. Atomic spectroscopy

During my master studies and at the beginning of the doctoral ones, I dealt with atomic spectroscopy, studying the intercombination transition  $5^1S_0 - 5^3P_1$  in cadmium. The aim of this work was to study the impact of collisions on the shape of the spectral line and theoretical models of the line shape. Measurements were performed using the laser induced fluorescence (LIF) method. The cadmium sample was placed in a quartz cell in a furnace at a temperature of about 700 K. The line hyperfine splitting in the <sup>113</sup>Cd isotope and the isotopic shift measured against the <sup>114</sup>Cd isotope were determined [3]. It has been shown that the collisional broadening coefficients of individual hyperfine components in the <sup>113</sup>Cd isotope perturbed by argon are different [2] and the presence of line asymmetry was observed, which was attributed to the effects related to the finite duration of the collision and line mixing [1].

### 3.4. Summary and perspectives

To sum up, in my work so far, I have aimed primarily at improving the precision and accuracy of measurements of the shape, positions and intensities of molecular lines, as well as at developing effective methods of analyzing the data obtained in these measurements. In recent years, there has occurred a significant progress: more and more often there are available in the literature line shape parameters that take into account subtle effects such as line narrowing or its asymmetry. The accuracy of the published data is also improving, which results from the development of measurement and computing techniques. The above-described works are part of this global trend. My research work has in particular contributed to:

- 1. The development of spectrometers enabling one of the most accurate measurements in molecular spectroscopy.
- 2. Obtaining consistency between the experimental and theoretical intensities of the spectral lines of carbon monoxide at a promille level, and carbon dioxide at the level of a few promille, i.e. an order of magnitude better than so far.
- 3. Establishing a long-term, fruitful collaboration between the theoretical and experimental groups.
- 4. Knowledge of the line-shape parameters of self-perturbed spectral lines of oxygen from the B-band with comparable accuracy as for the A-band, thanks to which they are almost ready for use in the most demanding atmospheric applications.
- 5. Construction of the first optical atomic clock in Poland, used in numerous applications in the field of metrology and basic research.

<sup>&</sup>lt;sup>89</sup>P. Wcisło et al., Nature Astronomy 1, 0009 (2017).

<sup>&</sup>lt;sup>90</sup>P. Wcisło et al., Science Advances **4**, eaau4869 (2018).

<sup>&</sup>lt;sup>91</sup>P. Krehlik et al., Astronomy & Astrophysics **603**, A48 (2017).

- 6. The development of a new measurement technique in an optical cavity, which enables accurate measurements of the spectral line intensities, and in saturation conditions one of the most accurate measurements of the line positions.
- 7. Obtaining the most accurate experimental dependence of the saturated vapor pressure of ice on temperature.

On the other hand, continuously improving measurement techniques and computational methods enable to ask questions that until recently could not be answered. They also enable to respond to at least some of the needs arising from the application of spectroscopic measurements, both practical ones related to basic research. The possibilities for setting new problems seem endless. My research plans include:

- Further studies of the B-band of oxygen. The work carried out so far at the Institute of Physics of the Nicolaus Copernicus University concerned mainly the parameters of self-perturbed oxygen lines, while in atmospheric applications, the line parameters corresponding to the perturbation by air are needed. Moreover, there are currently no experimental data on the dependence of the line-shape parameters in this band on the temperature. Work on determining these parameters is in progress. I also started research on the effects of collisionally induced absorption (CIA) in the spectral range corresponding to the B band of oxygen. The CIA is an effect important for the interpretation of atmospheric spectra for applications requiring the highest accuracy, however it is poorly understood so far.
- 2. Collaboration within the newly established Task Group on Advanced Spectroscopy within the Consultative Committee for Amount of Substance (operating at the International Bureau of Weights and Measures, BIPM) with gas metrology and spectroscopy teams. The aim of the group is to develop spectroscopic methods through rigorous comparative measurements, and to define standards for conducting spectroscopic measurements in which the amount of substance is determined.
- 3. Further collaboration with theoretical computing teams to obtain accurate line intensities for different molecular bands important for atmospheric and astrophysical research. In particular, further work is already underway on the carbon monoxide molecule, focusing on the intensities of the lines of very weak absorption bands, the so-called high overtone bands.
- 4. Measurements of the line-shape parameters in the high temperature range. Currently, I am involved in the construction of a spectrometer that will be adapted to measurements at temperatures up to about 300°C. It will enable measurements in a much wider range of temperatures than before, needed to interpret the spectra recorded for the purposes of astrophysical applications.
- 5. Over many years, an unsolved problem is the availability of accurate spectroscopic data on the spectrum of water vapor. It is a molecule with a complex spectrum. It is also a difficult experimental object due to strong adsorption effects on various surfaces. However, due to its structure, water absorption lines occur in all spectral ranges, affecting practically all atmospheric measurements. I plan to measure the intensity of the water absorption lines and collaborate with the UCL theoretical group to improve the existing spectrum model.
- 6. I also plan to measure the spectra of minor isotopologues of molecules such as oxygen and carbon monoxide. Research on them is difficult due to the problems associated with determining their content in a sample. Hence, there is no high-accuracy of data, which is also needed in the atmospheric research.

# 4. Presentation of significant scientific or artistic activity carried out at more than one university, scientific or cultural institution, especially at foreign institutions

My research activity so far has been carried out in two institutions: the Nicolaus Copernicus University in Toruń (NCU), which is the place of my employment, and the National Institute of Standards and Technology (NIST, Gaithersburg MD, USA). I have completed two internships at NIST, the scientific results of which are summarized below. My other scientific achievements are the result of work carried out at the Nicolaus Copernicus University.

### 4.1. National Institute of Standards and Technology, 09.2009 - 02.2010

During the above-mentioned period, I did an internship at NIST during my doctoral studies. I made there measurements of the dependence of the saturated vapor pressure of ice on the temperature, which were the basis of my doctoral dissertation and the last two publications from the list below. My internship at NIST in 2009-2010 resulted in the following publications:

- 1. D. A. Long, **K. Bielska**, D. Lisak, D. K. Havey, M. Okumura, C. E. Miller, J. T. Hodges, *The air-broadened*, *near-infrared CO*<sub>2</sub> *line shape in the spectrally isolated regime: Evidence of simultaneous Dicke narrowing and speed dependence*, J. Chem. Phys. **135**, 064308 (2011)
- 2. K. Bielska, D. K. Havey, G. E. Scace, D. Lisak, J. T. Hodges, *Spectroscopic measurement of the vapor pressure of ice*, Phil. Trans. R. Soc. A **370**, 2509-2519 (2012)
- 3. K. Bielska, D. K. Havey, G. E. Scace, D. Lisak, A. H. Harvey, J. T. Hodges, *High-accuracy measurements of the vapor pressure of ice referenced to the triple point*, Geophys. Res. Lett. 40, 6303-6307 (2013)

### 4.2. National Institute of Standards and Technology, 02.2012 - 08.2014

During my work at NIST, the experimental part of the work [H1] was done as part of the scientific achievement referred to in Art. 219 section 1 item 2 of the Act.

As a result of my work at NIST during the postdoctoral fellowship, the following papers were published:

- 1. D. A. Long, L. Gameson, G.-W. Truong, **K. Bielska**, A. Cygan, J. T. Hodges, J. R. Whetstone, R. D. van Zee, *The effects of variations in buffer gas mixing ratios on commercial carbon dioxide cavity ring-down spectroscopy sensors*, J. Atmos. Ocean. Tech. **30**, 2604–2609 (2013)
- J. Courtois, K. Bielska, J. T. Hodges, *Differential cavity ring-down spectroscopy*, J. Opt. Soc. Am. B: Opt. Phys. 30, 1486-1495 (2013)
- D. A. Long, A. J. Fleisher, K. O. Douglass, S. E. Maxwell, K. Bielska, J. T. Hodges, D. F. Plusquellic, Multiheterodyne spectroscopy with optical frequency combs generated from a continuous-wave laser, Opt. Lett. 39, 2688-2690 (2014)
- [H1] O. L. Polyansky, K. Bielska, M. Ghysels, L. Lodi, N. F. Zobov, J. T. Hodges, J. Tennyson, *High-accuracy CO<sub>2</sub> line intensities determined from theory and experiment*, Phys. Rev. Lett. 114, 243001 (2015)

# 5. Presentation of teaching and organizational achievements as well as achievements in popularization of science or art

### 5.1. Teaching at Faculty of Physics, Astronomy and Informatics NCU

### 5.1.1. Before PhD

- 1. 2007 2008:
  - (a) Matematyka elementarna [Elementary mathematics] (exercises) 4 groups
- 2. 2008 2009:
  - (a) Matematyka elementarna [Elementary mathematics] (exercises) 4 groups
- 3. 2009 2010:
  - (a) Elementy fizyki [Elements of physics] (exercises) 1 group
  - (b) Elementy fizyki [Elements of physics] (laboratory) 1 group
- 4. 2010 2011:
  - (a) Elementy fizyki [Elements of physics] (exercises) 1 group

### 5.1.2. After PhD

 $1. \ \ 2011 - 2012$ 

(a) Pracownia elektroniczna I [First electronic laboratory] (laboratory) 2 groups

### $2.\ \ 2014-2015$

- (a) Fizyka [Physics] (laboratory) 1 group
- (b) Fizyka i technologia próżni [Physics and technology of vacuum] (lecture) 1 group
- (c) Fizyka ogólna 3 fizyka falowa i optyka [Physics 3 wave physics and optics] (exercises) 1 group
- (d) Praca w zespołach badawczych [Work in research teams] (laboratory) 1 group
- (e) Fizyka ogólna III (optyka) [General physics III (Optics)] (exercises) 1 group
- (f) Matematyczne podstawy metrologii [Mathematical basics of metrology] (exercises) 2 groups
- (g) Podstawy elektroniki [Elementary electronics] (laboratory) 1 group
- (h) Pracownia obróbki danych pomiarowych [Measurement data processing laboratory] (exercises) 1 group
- 3. 2015 2016
  - (a) Fizyka i technologia próżni [Physics and technology of vacuum] (lecture) 1 group
  - (b) Fizyka ogólna 3 fizyka falowa i optyka [Physics 3 wave physics and optics] (exercises) 1 group
  - (c) Praca w zespołach badawczych [Work in research teams] (laboratory) 1 group
  - (d) Pracownia fizyczna 1 cz.1 [Physical laboratory] (laboratory) 1 group
  - (e) Matematyczne podstawy metrologii [Mathematical basics of metrology] (exercises) 2 groups
  - (f) Metody opracowywania danych [Methods of data analysis] (lecture) 1 group
  - (g) Metody opracowywania danych [Methods of data analysis] (exercises) 1 group
  - (h) Pracownia obróbki danych pomiarowych [Measurement data processing laboratory] (laboratory) 1 group
- $4. \ \ 2016 2017$ 
  - (a) Analiza matematyczna 2 [Mathematical analysis 2] (exercises) 1 group
  - (b) Fizyka i technologia próżni [Physics and technology of vacuum] (lecture) 1 group
  - (c) Fizyka ogólna 3 fizyka falowa i optyka [Physics 3 wave physics and optics] (exercises) 1 group
  - (d) Pracownia fizyczna 1 cz.1 [Physical laboratory] (laboratory) 1 group
  - (e) Pracownia fizyczna 1 cz.1 [Physical laboratory] (exercises) 1 group
  - (f) Matematyczne podstawy metrologii [Mathematical basics of metrology] (exercises) 2 groups
  - (g) Podstawy elektroniki [Electronics] (laboratory) 1 group
- 5. 2017 2018
  - (a) Podstawy elektroniki [Electronics] (laboratory) 1 group
  - (b) Podstawy metrologii [Basics of metrology] (exercises) 2 groups
  - (c) Pracownia zespołowa [Laboratory team] (laboratory) 1 group
- 6. 2018 2019
  - (a) Fizyka ogólna 3 fizyka falowa i optyka [Physics 3 wave physics and optics] (exercises) 1 group
  - (b) Pracownia fizyczna 1 cz.1 [Physical laboratory] (laboratory) 1 group
  - (c) Analiza matematyczna 1 [Mathematical analysis 1] (exercises) 1 group

- (d) Podstawy elektroniki [Electronics] (laboratory) 2 groups
- (e) Podstawy metrologii [Basics of metrology] (exercises) 2 group
- 7. 2019 2020
  - (a) Fizyka ogólna 3 fizyka falowa i optyka [Physics 3 wave physics and optics] (exercises) 1 group
  - (b) Analiza matematyczna 1 [Mathematical analysis 1] (exercises) 1 group
  - (c) Podstawy metrologii [Basics of metrology] (exercises) 1 group
- 8. 2020 2021
  - (a) Fizyka ogólna 3 fizyka falowa i optyka [Physics 3 wave physics and optics] (exercises) 1 group
  - (b) Analiza matematyczna 1 [Mathematical analysis 1] (exercises) 1 group
  - (c) Podstawy metrologii [Basics of metrology] (exercises) 1 group
- 9. 2021 2022
  - (a) Fizyka ogólna 3 fizyka falowa i optyka [Physics 3 wave physics and optics] (exercises) 1 group
  - (b) Analiza matematyczna 1 [Mathematical analysis 1] (exercises) 1 group
  - (c) Podstawy metrologii [Basics of metrology] (exercises) 1 group

### 5.2. Supervision over diploma theses

- 1. engineering thesis: Paulina Lubińska, "Budowa i zastosowanie interferometru Fabry-Pérot" [Construction and application of the Fabry-Pérot interferometer], technical physics, 2017
- bachelor thesis: Anna Macko, "Oprogramowanie do analizy i prezentacji wyników pomiarów kształtu linii widmowych" [Software for analysis and presentation of spectral line shape measurement results], physics, 2017

### 5.3. Supervision over PhD students

2019-present: co-supervisor of Aleksandr Balashov PhD project "Highly accurate line intensity studies of weak molecular transitions for atmospheric application"

# 5.4. Supervision over students within "The Toruń Astrophysics/Physics Summer program - TAPS"

Grzegorz Łukasiewicz, Jagiellonian University, 4 weeks. The student built a simple CRDS type spectrometer and tested its operation.

### 5.5. Talks presented during the Seminar of the Institute of Physics NCU

10.06.2021 "Molecular spectroscopy: towards accurate reference parameters for atmospheric applications"

# 5.6. Talks presented during the seminar of the Department of the Atomic, Molecular and Optical Physics

11.04.2008, "W poszukiwaniu struktury izotopowej linii widmowej 326,1 nm kadmu" [In search of the isotopic structure of the spectral line 326.1 nm of cadmium]

8.05.2009, "O białych komórkach i teorii Knota" [About white cells and the Knot theory]

5.03.2010, "Pomiar prężności par nasyconych lodu z wykorzystaniem spektroskopii typu FS-CRDS" [Measurement of saturated vapor pressure of ice using FS-CRDS spectroscopy]

11.03.2011, "Co wiemy o prężności par nasyconych lodu?" [What do we know about the saturated vapor pressure of ice?]

6.05.2011, "Spektroskopowe badania prężności pary nasyconej lodu" [Spectroscopic studies of the saturated vapor pressure of ice]

12.06.2015, "Differential cavity ring-down spectroscopy (D-CRDS)"

3.02.2017, "Pomiary natężeń linii widmowych dwutlenku węgla" [Measurements of the intensity of spectral lines of carbon dioxide]

16.04.2021, "Near-infrared saturation spectroscopy of CO in an optical cavity"

# 5.7. Council of the Faculty of Physics, Astronomy and Informatics and the Board of Disciplines of Physical Sciences

Since 2017, I have been a representative of academic teachers without the title of professor or degree of habilitated doctor in the Council of the Faculty of Physics, Astronomy and Informatics at the Nicolaus Copernicus University. Then, since the change in the structure of the University, I belong to the Board of Disciplines of Physical Sciences.

## 5.8. Open days - action "Dziewczyny do Ścisłych!"

In the academic years 2015/2016 and 2016/2017 I represented the Dean of the Faculty of Physics, Astronomy and Informatics for the campaign "Dziewczyny do Ścisłych!" [Girls to the Science!]. Its aim is to promote studying programs in the field of exact and technical sciences among female students of secondary schools. As a part of the campaign organized by the "Perspektywy" Educational Foundation under the patronage of the Conference of Rectors of Polish Technical Universities, I organized an "open day" at the Faculty.

### **5.9.** Other organizational work

Organizing an exhibition "70 lat fizyki na UMK" [70 years of physics at NCU] (2016).

### 5.10. Other activities promoting science

- 1. Exhibition "Fiat Lux od Witelona do tomografu optycznego" [Fiat Lux from Witelon to optical tomograph] in the Old Town Hall in Toruń participation in the organizing team, 2008
- 2. Lecture for teachers "Fizyczne właściwości wody. Przemiany fazowe, para nasycona lodu" [Physical properties of water. Phase transitions, saturated vapor of ice], I Liceum Ogólnokształcące in Toruń, 23.11.2011
- Organization of workshops for students of upper secondary schools "Nowoczesna Fizyka Atomowa, Molekularna i Optyczna dla Młodzieży II" [Modern Atomic, Molecular and Optical Physics for Youth II], Toruń, 28-29.09.2015

## 6. Other information about professional career

### 6.1. Prizes and awards

- 1. Team award of the Rector of the Nicolaus Copernicus University (2<sup>nd</sup> degree) for achievements in the field of science and research in 2012
- 2. "MML Accolade: MML Distinguished Associate for the development and application of advanced laser spectroscopy methods, enabling sensitive and accurate measurements of greenhouse gases", National Institute of Standards and Technology, Materials Measurement Laboratory, 2016