

Author's abstract

1. First name and surname.

Mirosław Zachwieja

2. Diplomas obtained, academic / artistic degrees – including the title, place and year of issue, and the title of doctoral thesis.

- 1987 Master of Science degree in physics obtained at the Department of Mathematics and Physics of the Pedagogical University in Rzeszów. The title of the master's thesis " Analysis of the Baldet-Johnson system band (1–0) in the $^{13}\text{C}^{16}\text{O}^+$ molecule spectrum"; thesis promoter: Prof. Ryszard Kępa, Ph. D..
- 1998 Doctorate degree in physical science obtained at the Department of Natural Science and Mathematics of the Pedagogical University in Rzeszów (currently the University of Rzeszów). The title of the doctoral thesis "Analysis of the $\text{A}^2\Delta\text{-X}^2\Pi$ system in the spectrum of $^{12}\text{C}^1\text{H}$ and $^{13}\text{C}^1\text{H}$ radicals"; thesis promoter: Prof. Ryszard Kępa, Ph. D.; advisers: Prof. Józef Szudy, Ph. D., The Nicolas Copernicus University in Toruń; Assistant Professor Jerzy Galica, Ph. D., Institute of Molecular Physics of Polish Academy of Science in Poznań; Prof. Marek Rytel, Ph. D., Pedagogical University in Rzeszów.

3. Information concerning employment in scientific / artistic institutions.

- 1987-1998 Assistant Lecturer at the Nuclear and Molecular Physics Unit (ZFAiM – Zakład Fizyki Atomowej i Molekularnej) of the Institute of Physics at the Department of Mathematics and Physics of the Pedagogical University in Rzeszów (currently the University of Rzeszów).
- 1998-2009 Assistant Professor in the Institute of Physics (ZFAiM) at the Department of Natural Science and Mathematics of the University of Rzeszów.
- 2001/2002 *Visiting Fellow* to the National Research Council of Canada (NRC / CNRC), Ottawa, Canada (scholarship NATO Science Fellowship, to conduct scientific research in the Steacie Institute of Molecular Sciences, team *Spectroscopy Group*, managed by

Dr. Benoit Simard) – 12 months (with a one-month break – at the scholarship half term – contact with family).

from 2009 Senior Permanent Lecturer in the Institute of Physics at the Department of Natural Science and Mathematics of the University of Rzeszów.

4. Indication of achievements* pursuant to article 16 item 2 of the act of law dated 14 March 2003, concerning scientific degrees and scientific titles, and degrees and titles in the domain of arts (Official Journal No. 65, item 595, with later amendments):

According to the aforementioned act of law, I wish to indicate the single subject cycle of 6 publications in the scope of optical molecular spectroscopy, applied in research of electronic-vibrational-rotational spectra, in the region of 200–900 nm of selected molecules and radicals. Each of the above mentioned publications is supplemented in the footnote with *impact factor* of the magazine, in accordance with the year of its publishing, number of quotations (according to the Web of Science database) and my personal estimated percentage contribution to the work.

a) title of scientific / artistic achievement,

"Precise high resolution spectrometric registration and analysis of electronic--vibrational-rotational spectra of selected molecules and radicals, with astrophysical significance (AlH, AlH⁺, ¹³C¹⁷O and CD)."

b) (author / authors, title / titles of publication, year of issue, name of the publishing house),

H1. W. Szajna, M. Zachwieja, "Emission spectroscopy of the A¹Π–X¹Σ⁺ system of AlH" — (2009), Eur. Phys. J. **D 55**, 549–555.

impact factor: 1.420; number of quotations: 3; my contribution to the work: 50%

H2. W. Szajna, M. Zachwieja, "The emission spectrum of the C¹Σ⁺–X¹Σ⁺ system of AlH" — (2010), J. Mol. Spectrosc. **260**, 130–134.

* In case of achievement accomplished by means of joint work / works, declarations of all its / their co-authors should be presented, stating their estimated percentage individual contributions

impact factor: 1.479; number of quotations: 2; my contribution to the work: 50%

H3. W. Szajna, M. Zachwieja, R. Hakalla, R. Kępa, "Emission Spectroscopy of AlH: the $X^1\Sigma^+$, $A^1\Pi$ and $C^1\Sigma^+$ States Characteristics" — (2011), *Acta Physica Polonica A* **120**, 417–423.

impact factor(2010): 0.467; number of quotations: 0; my contribution to the work: 40%

H4. W. Szajna, M. Zachwieja, "High-resolution emission spectroscopy of the $A^2\Pi-X^2\Sigma^+$ system of AlH^+ " — (2011), *J. Mol. Spectrosc.* **269**, 56–60.

impact factor(2010): 1.479; number of quotations: 1; my contribution to the work: 50%

H5. R. Hakalla, M. Zachwieja, "Rotational analysis of the Ångström system ($B^1\Sigma^+-A^1\Pi$) in the rare $^{13}C^{17}O$ isotopologue" — (2012), *J. Mol. Spectrosc.* **272**, 11–18.

impact factor(2010): 1.479; number of quotations: 0; my contribution to the work: 50%

H6. M. Zachwieja, W. Szajna, R. Hakalla, "The $A^2\Delta-X^2\Pi$ band system of the CD radical" — (2012), *J. Mol. Spectrosc.* **275**, 53–60.

impact factor(2010): 1.479; number of quotations: 0; my contribution to the work: 70%

c) description of scientific / artistic objective of the above work / works and accomplished results, including description of their possible use.

The scientific objective of the indicated works was to obtain possibly the most precise, high-resolution electronic-vibrational-rotational spectra of selected molecules, including radicals, and subsequently detailed analysis of these spectra, as well as determination of new or more detailed parameters of electronic-rovibronic structure of molecules under study. In order to achieve this, I built the world's most precise (as far as I am aware) dispersion spectrometer with reflective diffraction grating, equipped on the output with an interferometrically controlled photomultiplier tube at the range of 200–900 nm, operating in the single photon counting mode. From the time the largest telescopes began being equipped with type *echelle*¹ dispersion

¹ R. S. Ram, P. F. Bernath and K. H. Hinkle, Infrared Emission Spectroscopy of NH: Comparison of a Cryogenic Echelle Spectrograph with a Fourier Transform Spectrometer. *J. Chem. Phys.* **110**, 5557-5563 (1999).

spectrometers (with the echelle grating as the dispersive element, and with a cryogenically cooled high-sensitivity CCD detector) instead of the previously applied FTS Fourier Spectrometers (*Fourier Transform Spectrometer*), significance of dispersion devices has increased in spectroscopic research works. The device that I have built fills the gap between the *echelle* type spectrometers and the FTS type spectrometers – it is characterised by intermediate sensitivity and resolution ability, compared to both types of spectrometers, while absolute accuracy and precision of measurements of wave numbers of spectrum lines and their intensities within the visible range and ultraviolet, are equal to the best FTS type spectrometers.

The basic component of my construction is the two-metre PGS-2 Ebert type spectrograph (*Plane Grating Spectrograph*) with a reflective diffraction grating with a total number of grooves of 45,600 and an interferometrically He-Ne laser controlled cooled photomultiplier tube, operating in the single photon counting mode. The sampling slot of the photomultiplier tube, dimensions 0.035 mm width and 10 mm height, moves together with the instrument in a uniform manner along the focal plane of the spectrograph (where photographic plate used to be formerly installed), while the diffraction grating remains stationary during the operation of scanning of the spectrum. The interferometer that controls position of the photomultiplier tube slot is synchronised with the system that counts impulses from the photomultiplier tube during sampling t_p . Both devices are timed by the system clock (the same for both devices) at the frequency of 1 MHz, which eliminates the risk of desynchronisation of these two devices in measurements lasting even as long as several dozens of hours. During scanning of spectrum the interferometer measures the changing position of the slot at the t_p time in single sampling of the photomultiplier tube, as many as 64 times, and the average value of position is transmitted to the computer, which then forms one measurement point together with the number of counts registered by the photomultiplier tube at the t_p time (full scanning at the distance of 215 mm includes approximately 73,000 measurement points). While measuring the spectrum scanning step equals 3 μm (this is the distance covered by the photomultiplier tube slot during the t_p sampling time, this time being selected prior to scanning from among the available values: 50 ms, 100 ms, 200 ms, 500 ms, 1 s, 2 s, 5 s or 10 s). The scanning step is therefore significantly shorter than the pixel width in CCD detectors applied in *echelle* type spectrometers, which usually equals 25 μm in the most sensitive devices of that type, or 13 μm in case of instruments of lower sensitivity. For these reasons the resolving power of

M.Z.

the device designed by me and the precision of determination of wave number of spectrum lines, are several times better than those accomplished in *echelle* type spectrometers.

I have applied the Hamamatsu R943-02 photomultiplier tube to detect radiation in the spectrometer designed by me, which is cooled based on the Peltier effect, down to the temperature of below -30°C , and operates in the single photon counting mode, at the quantum efficiency of approximately 20% (i.e. on average every fifth photon coming into the detector produces an impulse and is subject to counting). The best cryogenically cooled CCD detectors applied in *echelle* type spectrometers, have efficiency of between 60–70%. Both types of detectors provide very high dynamics of measurements (photomultiplier tube – several times higher), which means that within the same spectrum being measured, intensity of lines recorded by my photomultiplier tube may differ even up to over 100 thousand times. Thanks to this it is possible to measure very low molecular spectra in presence of extremely strong atomic lines (for instance Ne) at the spectrum source. Such measurements are in practice impossible to be conducted with the use of FTS² spectrometers, since detectors applied therein do not ensure sufficient dynamics of light intensity measurements. The applied R943-02 photomultiplier tube is characterised by perfect linearity at the frequency of measurements up to 6 million per second (slowly increasing saturation occurs above this value). This enables retaining the ratio of intensity of registered lines during scanning, which in connection with interferometric control of locations of the photomultiplier tube's slot provides for perfect mapping of the scanned spectrum even in cases of partial overlapping of lines. In consequence, while analysing these spectra, this allows to obtain wave numbers of overlapping lines, which significantly extends the abilities of the spectrometer designed by me, especially that registered single lines have symmetric shape, half width of approximately $40\ \mu\text{m}$ ($0.15\ \text{cm}^{-1}$ in the region of $20,000\ \text{cm}^{-1}$) and properly describes with the Gauss contour.

The absolute accuracy of measurements of wave numbers of lines, at the level of $\pm 0.0015\ \text{cm}^{-1}$ (with values of wave numbers at $20,000\ \text{cm}^{-1}$) is ensured by the innovative method of calibration of measured spectrum, developed by me, in real time of scanning, instead of doing so before or after its completion, as it usually occurs in this type of spectrometers. Thanks to this method, all fluctuations of line positions are compensated

² D. Cossart, M. Elhanine, An advantage of the dispersive optical spectroscopy relative to that using Fourier transform application to the emission spectra of SiC, *Chem. Phys. Lett.* **285** (1998) 83-91.

during spectrum scanning, due to minimum changes of the diffraction grating position angle (caused by mechanical and thermal interferences) or due to changes of light refraction factor (caused by changing temperature, air pressure and humidity in the laboratory or inside the spectrograph itself). During the measurements conducted I use two sources of spectrum: one – generates the spectrum under study, the other – to provide the reference spectrum. Light is almost always projected onto the input slot of the spectrograph, from the examined source. Calibration lines (Th atomic lines) "appear" in the examined spectrum thanks to momentary deflection of light from the reference source onto the spectrograph input slot, at appropriate moments during scanning, via the computer controlled quartz prism. Each registered Th reference line occupies 80 μm of the examined spectrum, and this fragment is not registered. This causes several dozens of Th atomic lines to appear in the examined spectrum without overlapping of both spectra, as this normally occurs in this type of instruments, where permanent semi-transparent mirror or *beamsplitter* are applied, instead of an adjustable prism, to mix light from both sources. Obviously, the method of calibration applied in the instrument designed by me, requires an extremely precise knowledge of locations of the standard spectrum lines (Th atomic spectrum) at a defined setting of the spectrograph diffraction grating position angle. For this reason, I conducted registration of the Th reference spectrum at the final stage of construction of the instrument, for the diffraction grating position angle settings, within the range from 5° to 70° , in 2.5° increments. In order to obtain identical distribution of light along the photomultiplier tube slot, I conducted final calibration tests and corrections of settings of both sources (measured and reference sources), with the use of two identical HCL lamps (*hollow-cathode lamp*), thus acquiring absolute accuracy of calibration at approximately $\pm 0.0015 \text{ cm}^{-1}$ within the range $11,000\text{--}22,000 \text{ cm}^{-1}$ and approximately $\pm 0.0025 \text{ cm}^{-1}$ within the range $22,000\text{--}30,000 \text{ cm}^{-1}$. In the spectrum range above $30,000 \text{ cm}^{-1}$ absolute accuracy of calibration gradually decreases (due to absence of Th atomic lines in this range, calibration is executed with the use of Th lines obtained from other spectrum orders than the registration home order), and reaches the value of approximately $\pm 0.009 \text{ cm}^{-1}$ at the limits of vacuum ultraviolet ($50,000 \text{ cm}^{-1}$). Accuracy of the measured ν wave numbers of lines, calculated as $\Delta\nu/\nu$, throughout the entire range $11,000\text{--}50,000 \text{ cm}^{-1}$ amounts to approximately $1.0 \cdot 10^{-7}$ and is comparable to the most accurate FTS spectrometers.

My design dispersion spectrometer, as all instruments of this type, demonstrates enormous vulnerability to mechanical and thermal

deformations of its body, particularly the optical tube. Such vulnerability results from close relationship of line positions on the spectrograph output with changes of diffraction grating position angle setting. Rotation of the grating by an angle of 0.01° will cause the shift of the line positions on the spectrometer output by approximately $700\ \mu\text{m}$. Limitation of fluctuations of line positions to below $0.5\ \mu\text{m}$ (in the area of $20,000\ \text{cm}^{-1}$ this would translate into fluctuations of wave numbers of lines at below $0.0020\ \text{cm}^{-1}$) is therefore related with the necessity to maintain a stable setting of the grating position angle relative to the parabolic mirror (which is located at the end of a two-metre long optical tube) at the accuracy of over 0.00001° (one one-hundred-thousandth of a degree). This is an extremely difficult task to accomplish, since as it appeared during numerous tests of the instrument, only normal wandering of the experimenter near the spectrograph placed on original factory-made foundations, causes violent movement of lines by $5\text{--}15\ \mu\text{m}$, which is caused by deformations of the ceiling in the laboratory and minimum twists of the spectrograph body. At the same time, experimenter's body warmth (emission of the thermal radiation) causes non-uniform heating of the spectrometer body, slowly changing in time, minimum twisting of the instrument optical tube, which results in slow, a dozen-or-so minutes long, relocation of lines, at the speed of approximately $1.5\ \mu\text{m}/\text{min}$. In order to eliminate these very undesirable phenomena and to reduce fluctuations of locations of registered lines, the spectrometer has been placed on a 6-cm thick granite plate, which rests on steel C-shape rails fitted to the main wall (with thickness of 35 cm and many tons of weight), in the laboratory premises. These measures resulted in full elimination of mechanical twisting of the spectrometer body and problems related to it. At the same time, careful thermal insulation of the spectrometer, significantly reduced vulnerability of the spectrometer to ambient temperature changes and sources of thermal radiation in the laboratory room (experimenter, power adapters, radiators, etc.). Combined with precise temperature stabilisation in the laboratory (with the use of a continuous operation air conditioning system), this retarded and reduced thermal fluctuations of locations of lines registered by the spectrometer to the value of approximately $1.5\ \mu\text{m}/\text{h}$. Such small fluctuations (temperature drift) are fully compensated by means of the above mentioned calibration method of the spectrum in real time of scanning. The only source of measurement errors, which may cause certain problems, are changes of atmospheric pressure during scanning of spectra. Particularly disadvantageous are sudden air pressure changes and related sudden changes of light diffraction coefficient in the air residing in the laboratory

M.Z.

room and inside the spectrograph. These cause line positions to rapidly shift (by several microns), which are only partly compensated during calibration. In order to be able to make possibly the most accurate measurements it is necessary to conduct these at a relatively stable atmospheric pressure (pressure fluctuations should not be greater than ± 1.0 hPa).

The instrument designed and built by me – dispersion spectrometer with diffraction grating, seems to be – as I have already mentioned – the world's most accurate device of this type. The only similar instrument, known to be to date (of which I learnt already after having built my device) is used³ in The National Institute of Standard and Technology (NIST) in the USA, alternately with registration on photographic plates. Due to lack of interferometric control of the photomultiplier tube slot position, photometric measurements can be use only to measure intensity of registered spectrum lines, while lengths waves (or wave numbers) of lines are determined based on photographic recordings. My innovative dispersion spectrometer with interferometric control of photomultiplier tube slot position, has been described and used in all of the above quoted publications **H1–H6**, which constitute my scientific accomplishment, and the results obtained in individual papers are discussed below, together with detailed description of my contribution to these publications; please note that this description does not take into account the enormous work effort which I put into the project between 2006–2008, to design, build and calibrate the spectrometer.

[H1] This was the first instance that possibilities of the new dispersion spectrometer were used in the work. Absolute accuracy of line wave numbers was accomplished at approximately $\pm 0.0015 \text{ cm}^{-1}$ for the $A^1\Pi-X^1\Sigma^+$ transition of the AlH molecule, registered at the region of 18,000–25,000 cm^{-1} with theoretical resolving power R of 228,000. In order to produce the measured spectrum, water cooled aluminium hollow-cathode lamp, filled with a mixture of neon and ammonia NH_3 instead of hydrogen used as a standard in similar applications, obtaining thus stable and strong source of spectrum of the A-X system in AlH (constancy of lines intensities for approximately 4 hours of illumination, signal/noise S/N ratio: approximately 250:1 for the strongest 0–0 band). Four off-diagonal bands (0–1, 1–0, 1–2, 1–3) were registered for the first time since 1954. Reduction of the spectrum was conducted to molecular parameters of effective Hamiltonian, achieving standard deviation σ of the model match to

³ Description of the instrument can be found at the following web address
<http://www.nist.gov/pml/data/platinum/>

measurements at 0.0009 cm^{-1} for the band 0–0 and $0.0014\text{--}0.0037 \text{ cm}^{-1}$ for bands 1– v'' . Very weak perturbation of the $A^1\Pi$ state – level $v = 1, J = 5$ was detected and analysed, unnoticed previously⁴ during analysing band 1–1 of the A–X system, with the use of a one-metre high resolution FTS type Fourier spectrometer. Molecular parameters of the upper $A^1\Pi$ state for $v = 1$ were determined more precisely, also a full set of Λ –doubling constants was obtained for the first time, i.e. q_1 and q_{D1} , and consequently equilibrium constants $q_e, \alpha_{q_e}, q_{De}$ and $\alpha_{q_{De}}$.

My contribution to the work: design of the construction of the discharge lamp and determination of the operating conditions for the lamp (in collaboration with W. Szajna), registration and calibration of transition spectra under examination, modifications of proprietary computer programmes used to determine molecular parameters, analysis of data and preparation of results for publishing (in collaboration with W. Szajna), preparation of major part of text in chapter 2 (*Experimental details*), participation in final editing of the paper text.

[H2] The work registers the $C^1\Sigma^+ - X^1\Sigma^+$ transition spectrum (bands 0–0, 1–1, 1–2) of the AlH molecule in the range of far ultraviolet $42,000\text{--}45,000 \text{ cm}^{-1}$ with absolute accuracy of wave numbers of lines reaching $\pm 0.004 \text{ cm}^{-1}$ and the resolving power $R = 456,000$. The spectrum under examination was produced in a water cooled, modified discharge lamp of commonly known design⁵, with an open hollow aluminium cathode and two anodes, filled with a mixture of neon and ammonia, which results in a four times higher intensity of spectrum lines of the A–X system than in case of the discharge lamp applied in the previous work [H1], at even higher stability of fluorescent discharge (constancy of intensities of AlH lines lasting approximately 6 hours of illumination). Precise values of wave numbers of lines and rotational terms was accomplished. A theoretical model was adapted to wave numbers of the C–X transition line, using the Curl–Dane–Watson method, obtaining standard deviation of match equal to 0.0074 cm^{-1} for the band 0–0 and 0.010 cm^{-1} for bands 1–1 and 1–2. More detailed spectroscopic parameters of the $C^1\Sigma^+$ state were determined. The theoretically expected rotational perturbations $v = 0, 1$ in the $C^1\Sigma^+$ state were experimentally observed and studied for the first time.

⁴ R. S. Ram and P. F. Bernath, High Resolution Fourier Transform Emission Spectroscopy of the $A^1\Pi - X^1\Sigma^+$ System of AlH, *Appl. Optics* **35**, 2879–2883 (1996).

⁵ R. Bacis, A new source for the search and study of electronic molecular spectra: the composite wall hollow cathode (CWHC), *J. Phys. E: Sci. Instrum.* **9** (1976) 1081–1086.

My contribution to the work: design of the construction of the discharge lamp and determination of the operating conditions for the lamp (in collaboration with W. Szajna), registration and calibration of transition spectra under examination, modifications of proprietary computer programmes used to determine molecular parameters, analysis of data and preparation of results for publishing (in collaboration with W. Szajna), preparation of major part of text in chapter 2 (*Experimental details*), participation in final editing of the paper text.

[H3] The work registered 0–0 and 1–1 bands of the $C^1\Sigma^+ - A^1\Pi$ transition in the range of 20,000–21,500 cm^{-1} , and the 0–2 band of the $A^1\Pi - X^1\Sigma^+$ system of the AIH molecule with absolute accuracy of wave numbers of lines reaching $\pm 0.003 \text{ cm}^{-1}$ and the resolving power $R = 228,000$. The spectrum under study was produced in a water cooled aluminium open hollow-cathode lamp with two anodes, filled with a mixture of neon and ammonia. Reduction of spectrum was conducted to molecular parameters of effective Hamiltonian, achieving standard deviation σ of the model match to measurements at 0.0032 cm^{-1} for the band 0–2 of the A–X system, and $0.0060\text{--}0.0077 \text{ cm}^{-1}$ for bands of the C–A system. Combined calculation of the determined molecular parameters was conducted with those acquired in works [H1] and [H2], thus obtaining more detailed molecular constants of the three lowest located electron states of the AIH molecule. Values of rotational terms of the $A^1\Pi$ state, $\nu = 1$, and $C^1\Sigma^+$, $\nu = 0, 1$ were determined with more accuracy.

My contribution to the work: design of the construction of the discharge lamp and determination of the operating conditions for the lamp (in collaboration with W. Szajna), registration and calibration of transition spectra under examination, modifications of proprietary computer programmes used to determine molecular parameters, analysis of data and preparation of results for publishing (in collaboration with W. Szajna), preparation of major part of text in chapter 2 (*Experimental details*), participation in final editing of the paper text.

[H4] The work registered bands 0–0 and 1–1 of the $A^2\Pi - X^2\Sigma^+$ system of the AIH^+ molecule in the 27,000–29,000 cm^{-1} spectral region, with absolute accuracy of wave numbers of lines of $\pm 0.003 \text{ cm}^{-1}$ and resolving power $R = 320,000$. The spectrum under study was produced in a water cooled aluminium open hollow-cathode lamp with two anodes, filled with a mixture of neon and ammonia. A full rotational structure of the spectrum was achieved for the first time – 12 branches up to $J = 36.5$ – plus the study

revealed the reason for sudden disappearance of lines with higher J values. A theoretical model was adapted to wave numbers of the A–X transition lines, using the Curl-Dane-Watson method, obtaining standard deviation of match equal to 0.0037 cm^{-1} and 0.0044 cm^{-1} , for 0–0 and 1–1 bands, respectively. Anomalous Λ -doubling was observed and studied in the $A^2\Pi$ state, as well as perturbations of terms of this state. Precise molecular parameters of the $X^2\Sigma^+$ state were obtained, most of which were obtained for the first time. Values of the $A^2\Pi$ state terms were determined, $v = 0$, and the perturbed $v = 1$ level.

My contribution to the work: design of the construction of the discharge lamp and determination of the operating conditions for the lamp (in collaboration with W. Szajna), registration and calibration of transition spectra under examination, modifications of proprietary computer programmes used to determine molecular parameters, analysis of data and preparation of results for publishing (in collaboration with W. Szajna), preparation of major part of text in chapter 2 (*Experimental details*), participation in final editing of the paper text.

[H5] The work includes registration in the region of $19,000\text{--}21,500 \text{ cm}^{-1}$ 0–1 and 0–2 band of the Ångström system ($B^1\Sigma^+ - A^1\Pi$) in a very rare molecule $^{13}\text{C}^{17}\text{O}$ with absolute accuracy of wave numbers of lines at $\pm 0.002 \text{ cm}^{-1}$ and the resolving power $R = 228,000$ for the 0–1 band and $R = 182,000$ for the 0–2 band. The spectrum under study was produced in a water cooled steel open hollow-cathode lamp with two anodes, where carbon ^{13}C was placed inside the cathode, followed by the lamp being filled with oxygen $^{17}\text{O}_2$. Carbon was deposited through several dozens of fluorescent discharge in the lamp filled with helium and acetylene $^{13}\text{C}_2\text{H}_2$, after which the gas mixture was pumped out of the lamp and the lamp was filled with oxygen, attaining thus a stable source of the $^{13}\text{C}^{17}\text{O}$ molecule spectrum source (perfect stability of molecular lines intensities for approximately 6 hours of illumination and current not greater than 50 mA). A theoretical model was adapted to wave numbers of the B–A transition line, using the Curl-Dane-Watson method, obtaining standard deviation of match equal to 0.0029 cm^{-1} and 0.0013 cm^{-1} , respectively for 0–1 and 0–2 band. Precise values of molecular constants B and D of the $B^1\Sigma^+$ state were determined, and effective constants of the perturbed state $A^1\Pi$. Numerous observed rotational perturbations in the $A^1\Pi$ state were identified and studied in detail.

M.Z.

My contribution to the work: design of the construction of the discharge lamp and determination of the operating conditions for the lamp (in collaboration with R. Hakalla), registration and calibration of transition spectra under examination, modifications of proprietary computer programmes used to determine molecular parameters, preparation of major part of text in chapter 2 (*Experimental details*), participation in final editing of the paper text.

[H6] The work included registration in the 22,800–24,000 cm^{-1} region of 0–0, 1–1, 2–2 and 3–3 bands of the $A^2\Delta-X^2\Pi$ system of the CD radical, with absolute accuracy of wave numbers of the lines reaching $\pm 0.003 \text{ cm}^{-1}$ and the resolving power $R = 270,000$. The spectrum under study was produced in a water cooled steel open hollow-cathode lamp with two anodes, filled with helium and methane C^2H_4 . Stable spectrum of the CD radical was obtained with current not exceeding 50 mA (constancy of molecular lines intensities for approximately 6 hours of illumination). The obtained spectrum is characterised by high vibrational and rotational temperature (observed lines up to $J = 38.5$), at a relatively small Doppler extension of the lines. This is the most complicated spectrum I have ever come across. Almost 1,200 lines from four diagonal bands of the A–X system are projected onto the same spectral region, causing their great concentration and overlapping, which significantly hampers analysis of the spectrum. A laborious rotational and vibrational interpretation of lines, which occurred several stages, was successfully completed – lines of all 12 main branches of previously unknown 2–2 and 3–3 bands of the A–X system were recognised. The erroneous interpretation of an isolated group of lines at 4,319.7 Å was corrected (these derive from the 3–3 band instead of 2–2, as it was believed previously). Wave numbers of lines of 0–0 and 1–1 bands were determined, which are more accurate by an order of magnitude than values achieved during earlier observations. Reduction of the spectrum was carried out to molecular parameters of effective Hamiltonian, achieving standard deviation σ of the model match to measurements at 0.0032 cm^{-1} , 0.0036 cm^{-1} , 0.0066 cm^{-1} and 0.0088 cm^{-1} , respectively for 0–0, 1–1, 2–2 and 3–3 bands. Combined calculation of the currently determined parameters was conducted with those acquired from vibrational-rotational measurements, as well as purely rotational in the $X^2\Pi$ state, obtaining final molecular parameters of both combined states, of which many for the first time. Molecular parameters obtained for the $X^2\Pi$ state reproduce fundamental transitions of the CD radical with accuracy in excess of 100 kHz, and these also cause the previous smaller discrepancies related to

M.2.

molecular constants of the $X^2\Pi$ state to be removed. Almost all molecular parameters of the $A^2\Delta$ state were achieved for the first time, including Λ -doubling constants p_Δ and q_Δ , which in the vibrational state $v = 0$ amount to, respectively: $1.52(36)\cdot 10^{-7} \text{ cm}^{-1}$ and $-4.58(57)\cdot 10^{-9} \text{ cm}^{-1}$. These are the smallest values of parameters of the fine structure, that have ever been determined, and the Λ -doubling effect in the $A^2\Delta$ state of the CD radical is significantly smaller than the hyperfine structure of this state. Also a distinct deviations from the Born-Oppenheimer's approximation were found, and an electron isotopic shift was determined for the $A^2\Delta$ state, which equals $\Delta v_e = 32.105 \text{ cm}^{-1}$ and the shift independent of the nuclear mass coefficient, $\Delta U = 64.763(38) \text{ cm}^{-1}$, was also calculated.

My contribution to the work: design of the construction of the discharge lamp and determination of the operating conditions for the lamp, registration and calibration of transition spectra under examination, modifications of proprietary computer programmes used to determine molecular parameters, analysis of data, preparation of results for publication (in collaboration with W. Szajna), writing major part of the publication.

It should be emphasised that the presented cycle of publications could have been prepared exclusively thanks to use of the dispersion spectrometer designed and built by me, while the results achieved fully confirm the instrument's usefulness in research of spectra and the electronic-rovibronic structure of molecules in the gaseous phase. The molecular parameters of examined molecules and radicals determined in the works, will be certainly used in databases and programmes for simulation of spectra (as it has already occurred in the past); these will also constitute the reference point for theoretical models and calculation methods in quantum chemistry.

5. Description of other scientific and research (artistic) achievements.

Scientific publications listed in the Web of Science data base

(state as on 21 June 2012)

Total number of publications (articles): **26** (19 after having received the doctorate degree).

Total *impact factor* of publications, according to the list Journal Citation Reports (JCR), in conformance with the year of publishing: **36.419**

Number of quotations: **322**

Number of quotations, excluding self-quotations: **287**

Average number of quotations per one publication: **12.38**

M.2 -

Hirsch index #H: 9

Full listing of publications and conference reports is provided in Enclosure No. 3 (including requirements defined in the Regulation of the Minister of Science and Higher Education, dated 1 September 2011, Official Journal No. 196. item 1165).

Description of scientific career before having obtained the doctorate degree

I commenced my research work in February of 1987, under the auspices of Prof. Ryszard Kępa, PhD, as early as during my university studies, conducting registration and analysis of the previously unexamined spectrum and structure of the Baldet-Johnson's system in the $^{13}\text{C}^{16}\text{O}^+$ isotopomer. During the following two years I developed application software to analyse spectra and to determine, based on these spectra, molecular parameters of diatomic molecules. These programmes are constantly being modified by me for specific tasks, and are utilised by all scientific and academic employees of our Unit. At that time I also carried out tests of the measurement instruments (a PGS-2 grating spectrograph for photographic registration and an interferometric comparator for scanning of photographic plates), which was installed in our Unit. My work resulted in significantly more accurate measurements, thanks to detection and elimination of systemic errors introduced by the grating spectrograph, as well as reduction of random errors that had occurred in the comparator. This enabled further research to be conducted more accurately: these focused on electronic-vibrational-rotational spectra as well as on the energetic structure of selected molecules CH, CO and NO and their isotopic species – due to their great significance in physical chemistry, astrophysics, natural environment research and in medicine. Such research works conducted between 1990–1997 resulted in publication of 7 papers in renowned scientific magazines (6 in the USA and one in England), 13 conference reports on international scientific conferences (Enclosure No. 3), as well as in the doctorate thesis, which defined original and important extension of spectroscopic and quantum-mechanical information about the CH radical structure in its two isotopologues: $^{12}\text{C}^1\text{H}$ and $^{13}\text{C}^1\text{H}$. My original proprietary publication in 1995, which constituted the foundations for my doctorate, is continuously being quoted – 89 times to date, while the spectroscopic constants of CH and NO radicals, determined by me, are utilised, for instance in the data base and in the LIFBASE⁶ application software, for simulation of spectra of diatomic molecules.

⁶ J. Luque and D. R. Crosley, "LIFBASE: Database and spectral simulation (version 1.5)", SRI International Report MP 99-009 (1999)

Description of scientific career after having obtained the doctorate degree

After having obtained the doctorate degree I decided to extend the field of my research interest onto other molecules, and to become familiar with new methods of molecular spectroscopy, for instant laser. To accomplish that I developed a research project, which was approved both by the inviting institution (National Research Council of Canada), as well as by the commission that awards the NATO Science Fellowship scholarships, as a result of which, I went to Canada in 2001 for 12 months. In the research team *Spectroscopy Group* managed by Dr. Benoit Simard, I conducted electronic-vibrational-rotational tests of PH₂ and SiNSi molecule spectra, excited with the laser induced fluorescence LIF (*Laser Induced Fluorescence*) under the conditions of supersonic molecular beam. The gathered vast research material was studied and analysed after my return to Poland, to subsequently become the foundation for six conference reports and for one publication.

While analysing the SiNSi spectrum it appeared that the resolution (0.07 cm⁻¹) applied during registration, and the calibration accuracy (absolute value ±0.2 cm⁻¹, precision ±0.03 cm⁻¹) were insufficient to conduct full interpretation of the registered spectrum. Therefore, I prepared the next research project, which focused on high-resolution registration of the SiNSi molecule spectrum, CW laser induced under the conditions of supersonic molecular beam. I intended to carry out my research work in the USA within the framework of the Fulbright Scholarship, which I applied for in 2005, successfully completing all stages of the contest; ultimately I was not awarded the grant. At that time I decided that I would create a modern laboratory for high-resolution and high-accuracy electronic-vibrational-rotational molecular spectra tests, with possibly high absolute measurement accuracy of wave numbers of lines and their intensities – that laboratory was intended to be established on site at our Unit, to enable use by my younger colleagues. Between 2006 and 2008, despite very low funds allocated to our Unit, we managed to build the world's most accurate dispersion spectrometer for the range 200–900 nm. It was designed based on the PGS-2 grating spectrograph and on the interferometrically controlled cooled photomultiplier tube, operating in the single photon counting mode. The sampling slot of the photomultiplier tube, dimensions 0.035 mm width and 10 mm height, moves together with the instrument in a uniform manner along the focal plane of the spectrograph (where photographic plate used to be formerly installed), while the diffraction grating remains

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stationary during the operation of scanning of the spectrum (the scanning step amounts to 3 μm).

While developing the instrument we had to overcome a number of technical problems, associated most of all with the enormous vulnerability of this kind of spectrometer to mechanical, thermal and electromagnetic interference. Finally, at the end of the year 2008, the system was ready to register, it was only necessary to provide a proper source for synthesis of molecules (or radicals) under study, and to excite electronic-vibrational-rotational spectra. In order to accomplish that we made our own modifications to a known design⁷ of a cooled hollow-cathode lamp with two anodes, thus achieving an efficient and stable source of molecular spectra, excited by a fluorescent discharge. Three operating modes of the lamp, found by us, enable achieving highly-excited electronic-vibrational-rotational spectra of radicals and molecules CH, CH⁺, CD, CD⁺, AlH, AlH⁺, CO, CO⁺, plus their isotopic species, accurate registration of which, under the conditions of high resolution ability and detailed analysis, objective of which is to determine new or more precise molecular parameters of studied molecules and the structure of their electronic-rovibronic states, constitutes the core for work of the scientific and research team in our Unit.

Scientific and research plans in the nearest years

The newly built Centre for Innovation and Transfer of Technical and Natural Knowledge at the Rzeszów University (the scheduled commissioning and ramp up – December 2012), will house, amongst others the Molecular Spectroscopy Unit (within the Laboratory of Material Spectroscopy). The basic instrumental equipment of the unit, besides the dispersion spectrometer of my design, will be the Fourier transform spectrometer with high-resolution reaching 0.0035 cm^{-1} , for the range 1,850 – 50,000 cm^{-1} (the only instrument of this type in the country) as well as a position for examination of spectra under the conditions of supersonic molecular beam. This will allow, amongst others, to conduct studies of spectra of astrophysical significance molecules in the laboratory environment, in conditions close to those found out in the cosmic space. Adiabatic cooling of plasma down to the temperature of several degrees Kelvin, will also allow us to conduct studies of multi atomic molecules (their spectra in higher temperatures are too complicated to be interpreted). We are open to cooperation with other scientific and research centres both in Poland and abroad. We are currently cooperating, amongst others, with Prof. Jacek

⁷ R. Bacis, A new source for the search and study of electronic molecular spectra: the composite wall hollow cathode (CWHC), *J. Phys. E: Sci. Instrum.* **9** (1976) 1081-1086.

Krełowski, PhD., from the Centre of Astronomy at the Nicolas Copernicus University in Toruń, Poland. Prof. Włodzimierz Jastrzębski, PhD., from the Institute of Physics of the Polish Academy of Science in Warsaw, is already interested to make use of our instrumentation. I am convinced that the launch of the new laboratory will significantly contribute to scientific development of our centre.

Scientific stays abroad

2001/2002 National Research Council of Canada (NRC/CNRC), Ottawa Canada (NATO Science Fellowship scholarship to conduct scientific research in the Steacie Institute of Molecular Sciences, in the unit *Spectroscopy Group*, managed by Dr. Benoit Simard) – 12 months (with a one month break – at half term of the scholarship – contact with family).

Distinctions as a result of scientific research conducted

- 1998 2nd degree prize awarded by the Chancellor of the Pedagogical University in Rzeszów, for scientific achievements.
- 2001 NATO Science Fellowship scholarship obtained by way of a competition (12th prize out of 22 awarded) to conduct scientific research for a period of 12 months, entitled „*Spectroscopic investigation of metal-containing molecules*” at NRC/CNRC in Canada.
- 2007 Award of the Department of Mathematics and Natural Science Dean at the Rzeszów University, for achievements in scientific work.

Functions performed

- 2001 Member of the Council of the Institute of Physics at the Department of Mathematics and Natural Science of the Rzeszów University (I gave up the seat due to my scientific trip to Canada).
- 2010/2011 Acting as the Deputy Director of the Institute of Physics for Scientific and Financial Matters at the Department of Mathematics and Natural Science of the Rzeszów University.
- since 2011 Acting as the Deputy Manager of the Atomic and Molecular Physics Laboratory in the Institute of Physics at the Department of Mathematics and Natural Science of the Rzeszów University.
- since 2011 Acting as the Deputy Manager of the Material Spectroscopy Laboratory in the newly built Centre of Innovation and Transfer

of Technical and Natural Science Knowledge (Polish: CliTWTP – Centrum Innowacji i Transferu Wiedzy Techniczno-Przyrodniczej) of the Rzeszów University.

since 2010 Manager of the Molecular Spectroscopy Unit at the Molecular Spectroscopy Laboratory of the Centre of Innovation and Transfer of Technical and Natural Science Knowledge (Polish: CliTWTP).

Membership in organisations

since 2005 Member of the Polish Society of Agrophysics

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