Publishable Summary for 18SIB04 QuantumPascal
Towards quantum-based realisations of the pascal

Overview

Realisations of the pascal relied on piston gauges (also known as pressure balances) and liquid manometers containing toxic mercury, both of which measure force per area. Their performance however had remained essentially unchanged over the past few decades, and they suffer from practical and environmental limitations. This project developed photon-based standards, which determine the pressure via gas density using the gas law. Following the implementation of the redefined SI in May 2019, the uncertainty of the Boltzmann constant has been eliminated, so at a given temperature, photon-based standards promised primary measurements limited only by the accuracy of the quantum calculations. By improving these calculations for relevant gas parameters for helium and argon and by realising, further developing, and evaluating six different density-based methods to assess and realise gas pressures in the 1 Pa to 3 MPa range, this project paved the way for quantum-based realisations of the pascal in the EU. In the longer term, such primary standards could be miniaturised, providing faster and calibration-free pressure measurements for industry at a fraction of the present cost.

Need

Accurate and fast gas pressure measurements were needed to ensure control and safety in a variety of critical industrial processes. In addition, manufacturers of pressure sensors required reliable, fast and automated calibration, preferably for a wide pressure range depending on the particular application. Conventional methods for the realisation of the pascal were based on force per area with relative uncertainties of a few parts in 10^6 at 100 kPa and a few parts in 10^4 at 1 Pa and had remained basically unchanged over recent decades. Piston gauges started to replace mercury manometers due to their superior accuracy and lack of environmental hazards. However, the fact that weights need to be exchanged on the piston gauge during a calibration leads to drawbacks such as slowness, bulkiness, fragility and complexity of operation. For pressure measurements below 3 kPa, other methods involving static or continuous expansion of gases had to be used which significantly increased the effort required for operation.

The importance of overcoming these limitations had been identified as a strategic goal by the CIPM (Comité international des poids et mesures) the Consultative Committee for Mass and related quantities (CCM) and the EURAMET Technical Committees for Mass and related quantities (TC-M), and in several publications where optical quantum-based methods were proposed for calibration-free sensors. The drawbacks can be overcome by photon-based devices, that could become inherent primary pressure standards significantly outperforming conventional standards, and which can potentially be implemented as desktop or even as on-chip versions.

Two national metrology institutes, NIST (USA) and NIM (China), had invested significant resources in developing quantum-based pressure standards utilising Fabry-Pérot (FP) cavities. Further research and development were however required to address limiting effects such as outgassing, cavity deformation, gas permeation as well as thermal and temporal instabilities.

Due to the very wide range of pressures that needed to be addressed, it was not feasible for this to be covered by one technique alone. The potential of other quantum-based techniques to act as pressure standards such as superconductive microwave resonators, Rayleigh scattering, multi reflection interferometry, gas thermometry methods and absorption spectroscopy therefore also needed to be investigated and evaluated.

In addition, a prerequisite for developing quantum-based primary pressure standards was accurate knowledge of the thermodynamic and electromagnetic properties of the gas used, however the available information was often limited or insufficiently accurate.

Objectives

The overall aim was to develop novel quantum-based pressure standards based on optical, microwave and dielectric methods and to assess their potential with the aim of replacing existing mechanical based pressure standards. Therefore, the specific objectives of this project were:

1. To improve the accuracy and extend the working range of Fabry-Pérot refractometry quantum-based methods that have the potential to become primary standards of the SI unit of pressure, the pascal. The target uncertainties (k=1) and pressure ranges are 500 ppm in the range 1 Pa - 1 kPa and 10 ppm in the range 1 kPa - 100 kPa.
2. To improve the accuracy and evaluate the potential of alternative pioneering (non Fabry-Pérot based) quantum-based approaches and detection methodologies for the realisation of absolute and partial pressure standards, including superconductive microwave resonators, Rayleigh scattering, multi-reflection interferometry, gas thermometry methods, absorption spectroscopy of selected molecular species with very long optical pathways and modulation techniques, with target uncertainties (k=1) less than 500 ppm between 1 Pa and 10 Pa, less than 50 ppm between 1 kPa and 100 kPa, less than 500 ppm between 100 kPa and 1 MPa and less than 5 ppm between 1 MPa and 3 MPa, depending on the measurement technique.
3. To develop improved ab-initio calculations of the thermodynamic and electromagnetic properties (static and dynamic polarisability, diamagnetic susceptibility along with dielectric- and density virial coefficients) of He, Ne, and Ar and the electromagnetic properties (intensities of specific absorption lines) for CO and CO_2 of gases as needed to meet objectives 1 and 2. For gases other than He, the accuracy of the calculations (targeted uncertainty contributions of 1 ppm to 5 ppm at 100 kPa, equivalent to an improvement of at least a factor of 5) to be validated by comparisons with the results from experiments using He as a calibrating reference substance.
4. To demonstrate the performance of the methods (FP-based refractometers, Rayleigh scattering, multi-reflection interferometry, gas thermometry, superconductive microwave cavity) developed in objectives 1 and 2 by comparison with conventional primary absolute pressure standards such as pressure balances.
5. To facilitate the take-up of the technology developed in the project by end users, i.e. the scientific, metrological, and industrial communities and standards developing organisations.

Progress beyond the state of the art

The project took advantage of recent advances in optical, microwave and dielectric measurement techniques, combined with the outstanding progress of quantum-based calculations of gas properties, to develop novel, improved pressure standards.

Refractivity or permittivity Fabry-Pérot cavity-based techniques for the realisation of the pascal (Obj. 1)

NIST was the world leader in the development and utilisation of FP-cavity based refractometry for pressure assessment, with claimed relative uncertainties of 9×10^{-6} at 100 kPa and 2×10^{-3} at 1 Pa. This project has developed techniques to overcome many of the left limitations of FP-cavity based refractometry by minimising the influence of cavity deformations induced by pressure, thermal effects, and gas diffusion, developing standards for the assessment of pressure with relative uncertainties of 500 ppm in the 1 Pa to 1 kPa range and 10 ppm between 1 kPa and 100 kPa.

Alternative non Fabry-Pérot based techniques for the realisation of the pascal (Obj. 2)

No single technique was able to cover the extensive pressure range targeted here, hence it was necessary to investigate other techniques, alternative to FP-cavity based refractometry. Therefore, other quantum-based methods for pressure assessments have been developed, including a simple and compact device for gas density/pressure measurements based on Rayleigh scattering (RAY), an optical pressure standard based on a homodyne interferometer with one arm folded by a multi-reflection assembly (UINT), two different polarising gas thermometry techniques, dielectric-constant gas thermometry (DCGT) and refractive index gas thermometry (RIGT), a superconducting RIGT (S-RIGT) for use in the low-pressure range and absorption spectroscopy for the optical measurement of partial pressures. The achieved standard uncertainties were less than 500 ppm between 1 Pa and 10 Pa, less than 50 ppm between 1 kPa and 100 kPa, less than 500 ppm between 100 kPa and 1 MPa and less than 5 ppm between 1 MPa and 3 MPa, depending on the measurement technique.

Improved ab initio calculations for the thermodynamic and electromagnetic properties of gases (Obj. 3)

Ab-initio calculations of gas properties are a prerequisite to make these quantum-based methods primary, for example, the uncertainties in the calculations for helium contributed 1 ppm to the overall uncertainty of pressure assessments at 100 kPa. Gases other than He provide higher polarisabilities and thus higher sensitivities, but due to their complexity existing gas parameters data was insufficiently accurate. The thermodynamic and electromagnetic properties of He, Ne and Ar and the electromagnetic properties of CO and CO_2 have therefore been determined to enable a link between calculations of the thermodynamic and electromagnetic properties of gas species on the quantum level and macroscopic pressure determinations. On average the newly calculated theoretical values reduced the uncertainties by more than a factor of five as compared to the previous world's most accurate values for all addressed relevant gas parameters.

Demonstration of the performance of the novel and improved methods compared with conventional primary absolute pressure standards (Obj. 4)

The performance of improved FP cavity refractometry and alternative novel methods (Rayleigh scattering, absorption spectroscopy, and gas thermometry techniques) has been assessed by comparing them with conventional primary pressure standards such as pressure balances. In addition, a comparison was undertaken between conventional pressure standards using a portable optical refractometer, comparing different conventional pressure standards and demonstrating how well the portable optical refractometer worked as a transfer standard.

Results

Development of Fabry-Pérot cavity (FPC)-based techniques for the realisation of the pascal (Obj. 1)

Five different FP-based refractometers have been realized and scrutinized: single and double cavity systems, constructed using various types of spacer materials (glasses and metals), addressed by light of different wavelengths (ranging from 532 nm to 1.55 µm). As is shown by the extensive scientific production [2, 4-9, 11-14, 20, 21, 23], conference proceedings,[1,2,3] and reports and guides,[4,5,6,7] the consortium has made significant and crucial progress towards several important concepts that is of importance for the future development of FP-refractometry, primarily pressure-induced cavity deformation, control and assessment of temperature of the gas, and gas purity (permeability and outgassing), as well as further key developments of the gas modulation refractometry (**GAMOR**) methodology, which mitigates the influence of various types of disturbances (e.g., from length drifts and outgassing) and thereby made high-precision assessments possible.

Several important steps towards the targeted uncertainty (500 ppm for 1 Pa to 1 kPa and 10 ppm for 1 kPa to 100 kPa) have been taken. The best achieved expanded uncertainty in the 10 Pa to 25 kPa pressure range is better than targeted by objective 1 [13]. For this pressure range, these uncertainties are the so far best in the EU and to a large degree similar to the world best published values. Furthermore, it has been concluded that the system, when compared to the NIST-system, reached thermal equilibrium two orders of magnitude faster due to its smaller volume and higher thermal conductivity of the cavity spacer allowing for fast measurement that are significantly less affected by thermodynamic effects [21]. Moreover, by use of two GAMOR utilizing refractometers coupled to a common pressure reference, it has been shown that the refractometers can provide short-term precision on the 1 s time scale of 3×10^{-8}, which was an order of magnitude better than the corresponding stability of the pressure reference (DWPG) [14]. The obtained uncertainty was within the targets for a larger part of the pressure range (viz. 10 Pa – 100 kPa). For the minor 1 Pa to 10 Pa range a pressure-independent uncertainty-contribution of 5 mPa (k=1) was achieved, slightly above the targeted value of 500 ppm. It is anticipated that latter will be achieved soon by combining the benefits of the various realised systems. Otherwise, the objective was successfully achieved while several additional important concepts were addressed (improved or resolved).

[1] Proceedings (status and progress of the QuantumPascal project) https://doi.org/10.21014/tc16-2022.103
[2] Proceedings (thermodynamic effects in GAMOR up to 100 kPa) https://doi.org/10.21014/tc16-2022.117
[3] Proceedings (cicular comparison using a transportable refractometer) https://doi.org/10.21014/tc16-2022.137
[4] QuantumPascal design guide D1 (FP-based refractometry) https://doi.org/10.5281/zenodo.7786489
[5] QuantumPascal report D2 (performance of FP refractometers) https://doi.org/10.5281/zenodo.7786658
[6] QuantumPascal guide A114 (pressure-induced deformation in FPCs) https://doi.org/10.5281/zenodo.7501925
[7] QuantumPascal guide A143 (GAMOR: performance & implementation) https://doi.org/10.5281/zenodo.7786349

Alternative non Fabry-Pérot based techniques for the realisation of the pascal (Obj. 2)

The realised systems were specifically based on the following methods: Rayleigh scattering (**RAY**), multi-reflection interferometry (**UINT**), Dielectric Constant Gas Thermometry (**DCGT**), Refractive index Gas Thermometry (**RIGT**), superconductive RIGT (**S-RIGT**) and absorption spectroscopy (**TDLAS**). Their metrological performances were evaluated.[8] Jointly, the developed techniques provided the targeted uncertainties in the wide pressure range from 1 Pa to 3 MPa.

A simple and compact **RAY** system has been realized at INRiM covering the 1 Pa – 1 MPa pressure range. By a multi-step analysis, the influence of stray-light was reduced by five orders of magnitude. The system used a custom software (python) and comprised a custom temperature control [15]. An extensive characterization with three different gases: He, Ar, and N_2 evidenced a strong linear dependence between scattered light intensity and pressure with residuals within 400 ppm. The RAY system provided fast measurements for pressures up to 1 MPa with an accuracy better 500 ppm paving the way for simple and compact transfer standards (potentially at low cost). A new **UINT** system was realized and used for pressure assessments in the 100 Pa – 120 kPa range [28]. It comprised a custom pressure/vacuum apparatus, with a double-step temperature control ($u(T)$ < 3 mK) and a novel interferometer, whose measurement arm used two high-reflective flat mirrors on a spacer made of Zerodur. The geometric path length of the unbalance as well as the pressure-induced deformation have been assessed leading to relative standard uncertainties from 5.2×10^{-4} to 1.0×10^{-5} for pressures between 100 Pa and 10 kPa and 1.0×10^{-5} for pressures between 10 kPa and 120 kPa fulfilling the main goal of the targeted standard uncertainty of 10 ppm at 100 kPa. After checking the working equations, the **DCGT**-based standard achieved a standard uncertainty of 10 ppm for the pressure range 1 MPa to 3 MPa by using Ar in combination with the recent virials [19]. Based on accurate determinations of the static refractivities of He, Ne, or Ar a primary **RIGT**-based pressure standard was realized with standard uncertainties varying between 3.7 ppm at 100 kPa and 13 ppm at 1 MPa. The developed **S-RIGT** system based on copper with a Nb coating operated between 200 Pa and 20 kPa at temperatures below 10 K. A second system was realized to evaluate thermo-molecular effects, since significant deviations of the measured pressures occurred, which were probably caused by the consideration of the thermo-molecular corrections found in the literature. The preliminary uncertainty evaluation of the S-RIGT using He yielded a standard uncertainty of 0.2 Pa at 500 Pa and 8.2 Pa at 20 kPa, with a major contribution from thermometry, which can be substantially reduced in the future [27, 29]. To drive forward the realisation of **TDLAS**-based partial pressure standards the existing Herriott-cell based setup at PTB was further improved. This included two quantum cascade lasers working at the fundamental bands of CO and CO_2 at 4.6 µm and 4.3 µm respectively. External cavities were used to narrow the linewidth. Adding a liquid-based thermalization led to long-term stabilities of ±10 mK while measurements were performed with two SPRTs ($u(T)$ < 350 µk (k=1)). The objective was successfully achieved.

Improved ab initio calculations for the thermodynamic and electromagnetic properties of gases (Obj. 3)

Gas properties of He, Ne and Ar but also CO and CO_2 that were required to realise the standards developed in obj. 1 and obj. 2 were calculated *ab-initio* and experimentally verified, both with lowest uncertainties worldwide. The key property was the dynamic molar polarizability or refractivity $A_\varepsilon(\omega)$ which is the sum of the dominating static molar polarizability $A_\varepsilon(0)$, the corresponding dispersion $\Delta A_\varepsilon(\omega)$ (frequency dependence with influence in the low order of %) and the magnetic susceptibility A_μ (influence of some 10 ppm). To account for the interaction between multiple gas particles, the 2nd and 3rd dielectric virial coefficients b_ε and c_ε of the three noble gases were determined as well. Therefore, a novel path integral approach was developed for b_ε [3] and c_ε [18].

For He, the dipole polarisability was published [1] with very low uncertainty of less than 0.1 ppm while papers on improved values for A_μ, b_ε, and purely, quantum mechanically calculated values of c_ε will follow. A pioneering contribution accepted for publication was the development of the exact three-body polarisability tensor. Experimental probing of the virials was done by DCGT measurements [19]. Overall, the properties of He were improved significantly, so that they now contribute less than 1 ppm to pressure uncertainty even at 7 MPa!

For Ne and Ar, uncertainties of up-to-date *ab-initio* calculations for $A_\varepsilon(0)$ cannot compete with highly precise experimental values (standard uncertainties 2 ppm). Instead, the latter were used as a basis. To include the frequency dependence $\Delta A_\varepsilon(\omega)$, most precise calculations of the dispersion coefficients were performed for Ne [10] and Ar which corresponded to an improvement by more than one order of magnitude in uncertainty. Similar improvements were reached for A_μ (partially published for Ne, publication on the relativistic treatment

[8] https://www.ptb.de/empir2019/fileadmin/documents/empir/QuantumPascal/reports/QP_D4_update_08_Dec_2022.pdf

of Ne and Ar will follow). Thanks to these ground-breaking calculations, the overall refractivity $A_\varepsilon(\omega)$ for Ne and Ar is now available for a broad temperature and frequency range with relative standard uncertainties in the order of 10 ppm. New values for b_ε [3] and c_ε [18] were provided based on the available literature pair polarisabilities whereas they now also feature an uncertainty estimate and can be applied for a broad temperature and frequency range. Experimentally, the virial coefficients were determined for Ne and Ar ($u_r(b_\varepsilon) \approx 15$ %, [17]) by combined DCGT and expansion experiments.

World's most precise calculations on the 0.1 % level of the selected absorption line strengths for H_2O, CO, and CO_2 have been carried out using the MOLPRO package for the Dipole moment surface *ab-initio* points and the nuclear motion programs DUO for CO and DVR3D. The results agreed well with the experimental findings [22, 24]. One highlight was the new possibility to use infrared absorption spectroscopy and the calculated fundamental gas parameters in the sense of the redefined SI to replace the Pee Dee Belemnite standard for the $^{13}C/^{12}C$ isotope ratio [16]. The objective was successfully achieved.

Demonstration of the performance of the novel and improved methods compared with conventional primary absolute pressure standards (Obj. 4)

Various comparisons by different NMIs/DIs between conventional pressure standards (pressure balances, Force balanced Piston Gauge) or transfer standards and improved/developed methods in the objectives 1 and 2 have been performed.[9] The latter were Fabry-Pérot cavity-based refractometers in the range 1 Pa to 100 kPa [13], Dielectric-Constant Gas Thermometry (DCGT) in the range 1 MPa to 3 MPa, Refractive Index Gas Thermometry (RIGT) in the range 100 kPa to 1 MPa, absorption spectroscopy (TDLAS), superconductive microwave resonators (S-RIGT) in the range 200 Pa to 200 kPa and unbalanced multi-reflection homodyne interferometer (UINT) in the range 400 Pa to 120 kPa. The different comparisons carried out showed that the developed new quantum-based instruments utilising various pressure measurement techniques had been successfully realized. Further work will be required to verify their performance in terms of accuracy and stability (short and long-term) and to extend the pressure range.

During this project the world's first transportable optical pressure standard (TOP) has been developed and was used successfully in a circular comparison. It is using the GAMOR methodology (introduced in Obj. 1) and was compared to a similar stationary optical pressure standard (SOP) as well as to conventional piston gauges. The TOP was packed on a standard EUR-pallet (300 kg) and successfully transported by truck from Borås in Sweden to Berlin in Germany, to Turin in Italy, to Paris in France, and back to Borås for a final comparison. Despite the adverse conditions during the chosen way of shipping, such as shocks or temperature influences, the TOP was able to be run with little effort after each transport and retained its performance during the whole comparison campaign. All pressure balances used at the different NMIs/DIs agreed well within their respective uncertainties for pressures above 20 kPa, while some discrepancies were seen at 10 kPa. In conclusion, the developed TOP was clearly suitable for the circular comparison and can be employed in future comparisons of conventional standards.[10] The objective was successfully achieved.

Impact

The consortium published over 29 peer reviewed articles in international journals, while more have been accepted for publication as well as drafted. It came to two successful dissertations and the consortium members had 20 presentations of their results in international and national conferences (IVC-21, 26th Colloquium on High-Resolution Molecular Spectroscopy HRMS 2019, 66th AVS International Symposium and exhibition à Columbus, Warsaw Molecular Electronic Structure virtual conference 2020, and DKD annual meeting 2019). There was training to higher education students on vacuum physics and metrology and research topics in physics. The established 'QuantumPascal' website of the project to make available general and detailed information and will continue to be maintained beyond the end of the project.

Impact on industrial and other user communities

Certainly, the developed and improved pressure standards will provide a major economic benefit to calibration laboratories and sensor and instrument manufacturers. The innovative approaches with the potential to perform automated calibrations between 1 Pa to 3 MPa aroused the interest of industrial stakeholder because the previous portfolio of available methods was small and calibrations in this pressure range were only covered by a combination of relatively time-consuming methods which led to higher costs for the end users.

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[9] https://www.ptb.de/empir2019/fileadmin/documents/empir/QuantumPascal/reports/QP_D7_update_08_Dec_2022.pdf

[10] QuantumPascal report D8 (circ. comparison with transport. refractometer) https://doi.org/10.5281/zenodo.7786697

The active dissemination of the results in the form of presentations, workshops and one-to-one meetings had led to the fact that not only the accredited laboratories are well prepared for a dissemination of the new quantum-based Pascal, but also at least the three largest European manufacturers of pressure measuring equipment and sensor instrumentation that rely on highly accurate pressure measurements have started corresponding activities in the form of feasibility studies, planning and, in some cases, production.

Impact on the metrology and scientific communities

The metrology and scientific communities have been and will be the first to benefit from the project's outputs. As a consequence of the revision of the SI in May 2019, in which the uncertainty of the Boltzmann constant k_B was eliminated, it is advantageous to realise the pascal for the given range through number density measurements to be more accurate and versatile.

The consortium liaised closely with the key metrological bodies (CIPM CCM, its working group on pressure and vacuum WGPV and the EURAMET TC-M) to present the developments within the project and get their direct feedback. This active engagement of these key stakeholders was part of the plan to ensure that the outcomes of the project will be disseminated worldwide to NMI laboratories and subsequently to any user who needs improved, traceable measurements of pressure, thus enabling broad industrial uptake. Accordingly, there were competing developments and, more importantly, synergies related to developments at other NMIs (e.g., NIST, NIM, NMIJ). Also, within Europe, other NMIs (CMI and TUBITAK) have been inspired by the results of this project and want to push the dissemination of quantum-based pressure standards. And as a bonus, the improved pressure standards and methods developed in this project also had impact on other fields of metrology, in particular primary thermometry and interferometric-based dimensional metrology.

Scientific impact is expected for the future from the application of the experimental methods developed within the project to extremely accurate, SI traceable determinations of the permittivity and the refractive index of pure gases and mixtures. The technical improvements led to advances in the field of optical cavity design. Furthermore, significant advances in the fields of atomic and molecular physics are expected by the future combination of refractometry and absorption spectroscopy, leading to highly accurate determination of absorption line strengths, for example, in the context of non-contact gas thermometry using spectroscopy. Particular benefits follow from the improved gas properties of neon and even more argon. Their higher measuring effect compared to helium can now be exploited in all kinds of gas metrology.

Impact on relevant standards

The development of photon-based measurements was still at an early stage hence no documentary standards have been affected directly. It is planned that once the novel measurement standards are established, existing documentary standards on vacuum gauges will be adapted to also account for the quantum-based methods and in the longer term, to develop standards analogous to existing standards on vacuum gauges for the quantum-based methods. In preparation for possible changes to existing standards and the development of emerging standards the ISO TC 112 "Vacuum Technology" received reports on the results achieved.

Longer-term economic, social and environmental impacts

This project further paved the way to the realisation of the vacuum scale in terms of density instead of pressure, while for most vacuum applications the density of gas molecules is the crucial quantity. The project helped to meet the growing demand from industry for high accuracy pressure and vacuum calibration services in Europe, whilst developing calibration procedures that are less time consuming. Vacuum and pressure related processes are key to many industrial applications that require very clean and well-controlled environments, such as semiconductor, photovoltaic, lighting, nanotechnology, surface engineering, pharmaceutical developments and food packaging. Better control of the vacuum and pressure processes will lead to improved cost efficiency, better overall environmental control over the complete process (higher quality products, fewer rejections), and hence increased profit margins and reduction of waste for the stakeholders.

The European vacuum and pressure industry are at the forefront worldwide, with a number of companies in Europe manufacturing pressure gauges, vacuum pumps and process tools. The introduction of optical measurement techniques led and will lead to the development of new technology of optical vacuum gauges that are less expensive than the primary ones. It is highly probable that these will be self-calibrating and require less maintenance. In the long run, this will enable manufacturers to produce a completely new generation of vacuum gauges that are more precise and in the long term more economical.

There will be advantages for aviation transport, where the height of an aircraft is measured by an altimeter that is based on an absolute pressure measurement. Further reduction in the standard vertical separation of aircraft will be needed in the future, which will increase the demands on the accuracy of pressure measurements. Not only will manufacturers of avionic measurement equipment and the aircraft industry benefit directly from the enhanced measurement capabilities at the NMI level, but the technology developed also has the potential to be directly utilised in future avionic pressure measurements, thus, supporting future transport demands.

For power plants and the storage of nuclear and toxic waste, it is crucial to reliably assess gas pressure due to strict requirements on safety and sterility. The developments achieved in this project will in the longer term provide more accurate means to monitor the operational conditions and will hence contribute to safer and more efficient conditions at power plants and critical facilities that handle toxic substances. Public agencies involved in environmental monitoring of atmospheric parameters and air pollution will profit from the improvements in absorption spectroscopy, which will lead in the longer term to the extremely accurate determination of the concentration of greenhouse gases, and hence have a significant effect on the detection of polluting sources and the improvement of climate models. Finally, the measurement of differential pressure is important for climate control in critical environments such as cleanrooms, hospitals, and biological/medical research laboratories. However, an additional 1 Pa of differential pressure in a medium-sized cleanroom requires around 3000 kWh of additional energy per year. More accurate differential pressure measurements would therefore contribute to reducing energy consumption in this environment.

List of publications

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[3] G. Garberoglio and A. H. Harvey. *Path-Integral Calculation of the Second Dielectric and Refractivity Virial Coefficients of Helium, Neon, and Argon*. Journal of Research of the National Institute of Standards and Technology, **125**, 125022, pp. 1-24 (2020) https://doi.org/10.6028/jres.125.022 (supplementary data set: https://doi.org/10.18434/M32225)

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<table>
<tr><td colspan="2">Project start date and duration:</td><td>1 June 2019, 42 months</td></tr>
<tr><td colspan="3">Coordinator: Tom Moses Rubin, PTB Tel: +4930 3481 7210 E-mail: tom.rubin@ptb.de
Project website address: https://www.ptb.de/empir2019/quantumpascal/home/</td></tr>
<tr><td>Internal Funded Partners:
1. PTB, Germany
2. CEM, Spain
3. CNAM, France
4. IMT, Slovenia
5. INRiM, Italy
6. LNE, France
7. RISE, Sweden</td><td>External Funded Partners:
8. FBK, Italy
9. UCL, United Kingdom
10. UmU, Sweden
11. UW, Poland</td><td>Unfunded Partners:
12. WIKA, Germany</td></tr>
<tr><td colspan="3">RMG: PTB, Germany (Employing organisation); CEM, Spain (Guestworking organisation)</td></tr>
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