Report of the CCQM and the Ad-Hoc Working Group on the Mole to the 25th meeting of the CCU, 21-23 September 2021

1. EXECUTIVE SUMMARY

Since the redefinition of the SI units at World Metrology Day on 20 May 2019, the SI is based on fundamental constants, the defining constants and, for the first time, on the number of elementary entities in case of the mole. The definition is now free of artefacts such as the kilogram prototype or any advice on how to realize the units. The wording of the new definition is now[1]:

"The mole, symbol mol, is the SI unit of amount of substance. One mole contains exactly 6.022 140 76 × 10^{23} elementary entities. This number is the fixed numerical value of the Avogadro constant when expressed in the unit mol^{-1} and is called the Avogadro number.
The amount of substance, symbol n, of a system is a measure of the number of specified elementary entities. An elementary entity may be an atom, a molecule, an ion, an electron, any other particle or specified group of particles."

The primary realization of the mole using the counting of entities is now further described in the mise en pratique of the mole along with the specific requirements for primary realizations in different fields of chemistry[2].
Further information about the relation of the new definition of the mole to the other SI units can now also be found in the 9th Edition of the SI Brochure along with similar information about the other SI units[3].
Achieving the redefinition in this form is the result of a very close cooperation between the Ad-hoc WG on the Mole of the CCQM and IUPAC who were seeking for a practical and easy-to-teach definition. This was accompanied by the trustful cooperation with CCU that recognized the specific requirements of the chemical community.

2. SCIENTIFIC, ECONOMIC AND SOCIAL CHALLENGES

Even after the redefinition of the SI and the mole, metrology needs to adapt to an ever-increasing accuracy of measurement and to new measurement challenges particularly in chemistry and biology. This is especially true for measurements that involve counting and quantifying more complex entities such as proteins, viruses, cells and their interaction.

Often, not even the required information for the relevant practical application is clear. For example, the detection and quantification of the status of health may result from measurements of, e.g., biomarkers or cells, but may also require metrological information about biomarkers attached to the cell, information about the degree of maturity of cell development or the vitality of a cell.

Quantitative information about the state of immunity is crucial in pandemic times but requires complex information about, e.g., antibodies and T-cells. It remains to be seen if and how this can be measured and expressed in an SI-traceable manner.

3. VISION AND MISSION

- to assure the worldwide use of the SI and the mole in particular in measurements by all stakeholders in chemistry and biology.
- to assure access to all relevant information about the use of the SI and the mole on all levels.

- to integrate all measurands and new aspects of measurement in chemistry and biology into the SI whenever possible in close collaboration with other consultative committees including the CCU.

4. STRATEGY

- to keep the *"mise-en-pratique"* for the realization of the mole at the *state-of-the-art*
- to create awareness with respect to the redefinition of the mole, explain reasons for the definition and prepare opinions for discussion in the CCQM.
- to address and discuss fundamental consequences of the redefinition also in collaboration with other consultative committees including the CCU.
- to discuss and integrate consequences of new measurement approaches in chemistry and biology with respect to the mole.

5. ACTIVITIES TO SUPPORT THE STRATEGY

A missing information to understand and teach the redefinition of the mole in its current form was a summarizing description of the background that led to the redefinition. This description should also include a representation of the enormous experimental research effort that was needed to fix the Avogadro constant with sufficient accuracy to safeguard continuity of measurement results before and after the definition.
Among other things this was achieved by a joint publication of the Ad-Hoc Working Group on the Mole including IUPAC that was published in Metrologia and summarized the redefinition process and the experimental efforts that made it possible[4]. In the meantime, this article has been downloaded about 8 000 times clearly indicating the need for such an explanation and its impact. Further activities to specifically address the wider community in chemistry were made. An editorial paper for "Analytical Chemistry", one of the most frequently read scientific journals in chemistry, has just been submitted.

5.1. PROGRESSING METROLOGY SCIENCE

Another consequence of the redefinition of the mole in its present form is an upcoming discussion about quantized measurements in general. Not only the mole, but also other quantities such as the electrical current or the mass can be measured by counting or even by counting entities. It is also a common process in other areas such as medicine (cell counting) or even with car exhaust measurements where soot particle counting has replaced analogue measurements (optical density) and is already required by law and subject to CCQM comparisons.
This upcoming importance of counting and its relationship to the SI units requires further consideration as to its proper and harmonized use in metrology and its terminology.
This aspect shall be discussed in future workshops of the working group jointly with CCQM and other consultative committees such as CCU.

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[1] SI Brochure: Le Système international d'unités; The International System of Units, 9th edition 2019; Bureau International des Poids et Mesures, ISBN 978-92-822-2272-0;
[2] https://www.bipm.org/en/publications/si-brochure/ (accessed June 21 2021).
SI Brochure-9th edition (2019) Appendix 2, *Mise en pratique for the definition of the mole in the SI*, Consultative Committee for Amount of Substance – Metrology in Chemistry and Biology (CCQM);
[3] SI Brochure: Le Système international d'unités; The International System of Units, 9th edition 2019; Bureau International des Poids et Mesures, ISBN 978-92-822-2272-0;
[4] Güttler, B.; Bettin, H.; Brown, R. J. C.; Davis, R. S., Mester, Z.; Milton, M. J. T.; Pramann, A.; Rienitz, O.; Vocke, R. D.; Wielgosz, R.I. *Metrologia*, **2019**, 56, 044002.