New defined units for chemistry – exactly!

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Explosion protection and metrology are both pivotal subjects of work at the Physikalisch-Technischen Bundesanstalt (PTB). According to the Einheiten und Zeitgesetz (units and time act), PTB is the National Metrology Institute of Germany and responsible for all aspects related to the realization, maintenance and dissemination of the legal units and their consistency with the international system of units (SI). New technologies and increasing demands from industry and society are constant challenges to the performance of measurement results and the SI. This fostered the evolution of the SI towards abstract definitions of its base units that are independent of the practical realization of the units. A revision of the SI was, therefore, enacted by the General Conference for Weights and Measures (CGPM) in May 2019.

Following a vision of Max Planck, four of the seven SI base units were redefined in the "new SI", - kilogram, ampere, kelvin and mole - based on natural constants, the so-called "defining constants". They are now based on invariable quantities for Planck constant (h), elementary charge (e), Boltzmann constant (k_B), and Avogadro constant (N_A). This ensures continuity over time. The practical realization of the base units on the highest metrological level is now described in accompanying documents, the *mises en pratique*.

Among those units the mole as unit for the base quantity "amount of substance" has special importance for chemistry. The first definition of the mole as an SI base unit in 1971 established a direct relation to another SI base unit, the kilogram, the unit for mass (via 12 g of the carbon isotope ^{12}C). This allowed for an easy route to the SI by measurement of the mass and established a simple relation between a macroscopic measurement and a microscopic number of entities via the molar mass constant. A big problem of this approach was, however, that the kilogram, as the last base unit in the SI, was still defined by an artefact, the international prototype kilogram (IPK), that was bound to change over time (and was known to do that!).

In the "new SI" the mole is now defined via a fixed value of the Avogadro constant and completely independent of the kilogram. A prerequisite for this redefinition was the determination of the Avogadro constant in the "old SI" with an unprecedented accuracy to maintain continuity of measurement results between the old and the new SI. The method used for this redetermination of the Avogadro constant is also the basis for the practical realization of the mole on the highest level of accuracy in the new SI and described in the *mise en pratique* of the mole. It is based on counting ^{28}Si atoms in a ^{28}Si enriched Silicon crystal by volumetric and X-ray interferometric measurements. A wealth of detailed information was needed to achieve the required accuracy for the redetermination of the Avogadro constant. Of special importance was the determination of the molar mass of the enriched Silicon. The relative measurement uncertainty is better than 2×10^{-8}.