

## METROLOGY IN CHEMISTRY (MiC) IN INDIA AND QA/QC FOR TRACE GASES & AEROSOLS MEASUREMENTS

**Prabhat K. Gupta**

Scientist 'F' & Head, Analytical Chemistry Section  
National Physical Laboratory, New Delhi

National Physical Laboratory (NPL) is the National Metrology Institute of (NMI) of India charged with the responsibility of realizing, maintaining and upgrading the Base and derived units' measurements at the apex level. As a signatory to the meter Convention India is committed to remove the Technical Barriers to Trades (TBT). To achieve this goal members nations of the Meter Convention have signed a Mutual Recognition Arrangement (MRA) on equivalence of national standards and measurement capabilities. NPL at present maintains standards for six base units only. One of the base units namely amount of substance SI 'mole' is at present being not realized at NPL. It is neither possible nor necessary to realize this unit directly in the laboratory and the exception is current international efforts to re-determine the Avogadro constant from measurements of the mass of a highly pure silicon artifact. However, it requires ultra-high accuracy isotopic measurements of amount ratios of Si isotopes to  $10^{-5}$  reproducibility on the ratio measurements and calibrating the results by synthetic isotope mixtures prepared to  $2 \times 10^{-5}$  relative combined uncertainty. This has opened the way to the establishment of 'Primary Standards of Measurements' for gas isotopic measurements. It can also combined with isotope dilution and it opens up a new route towards a realization of traceability of an amount-of-substance measurement to the SI and to the (measurement procedure and instrumentation leading to) Avogadro constant. This physical route to realize SI mole is extremely expensive and still not achievable by advance countries. The absence of a direct realization of mole is the cause of many of the conceptual difficulties encountered when making practical measurements of amount of substance that is traceable to the SI.

Some methods combine measurements made in SI units, such that the result is an amount of substance correctly expressed in moles. This is the essential property of primary methods. The results of a measurement made at the end of a chain of comparisons linked to a primary method fulfill the definition of traceability applied to the SI as stated in the International Vocabulary of Basic and General Terms in Metrology (VIM) [7, para. 6.10]: "Property of the result of a measurement or the value of a standard whereby it can be related to stated references, usually national or international standards, through an unbroken chain of comparisons all having stated uncertainties". Measurements of Amount of Substance occurs largely, but not exclusively, in chemistry and is used when a quantity is required that characterizes a number of entities. The accepted symbol for the quantity *amount of substance* is 'n', and the name is sometimes abbreviated to the single word *amount*. When the material is known, the words "amount of substance" are usually replaced by the specification, for example, "amount of sodium chloride". Amount of substance is an extensive quantity (whose magnitude is additive for subsystems) and its unit, the mole, is never realized directly. Measurements of amount of substance are usually combined with other extensive quantities such as volume, V, or mass, m, to derive intensive measures such as concentration,  $c = n/V$  or amount content,  $k = n/m$  which have units of mol/m<sup>3</sup> or mol/kg. In other cases, two measurements of amount of substance are

combined to measure amount ratio or amount fraction, which have units of mol/ mol. As a method that gives a result in moles per unit volume or moles per unit mass can be obtained with a traceable measurement of volume or mass to yield an extensive measurement of amount of substance in moles. Metrology in Chemistry (MiC) involves the determination of accurate amounts of substance by use of definitive methods such as Gravimetry, Titrimetry, Coulometry and pH etc. NPL being at the apex of the chain of traceability in the country and through its linkage with BIPM, it is to ensure traceability to international standards.

MiC will now have major thrust in coming five year plan of NPL and is vital to enhance quality management system for chemical measurements in the country. It envisages to establish and realize seventh SI base unit: the amount of substance 'mole', through MiC, create the related facilities and capacity building at apex level and establish a nation-wide network, for national traceability and improving upon the uncertainty for various parameters and having its linkages with Certified Reference Materials (CRM) programme and participation in international key-comparison programme in MiC areas organized by CCQM of BIPM (Paris), APMP etc. including the bilateral comparisons & collaborations with other advanced NMIs.

Effort are being made by NMIs world over to realize the SI unit mole, through chemical routes by MiC, in the areas of organic/ inorganic/ gas/ electrochemical/ surface & bio analysis, because of its tremendous scope touching all aspects of life viz. energy sector, health & environment, food security, drinking water, trade, and societal. To create Indian MiC network of laboratories, for development and validation of MiC procedures, training of manpower, linkages with Certified Reference Materials (CRM) programme for various MiC areas viz. CFTRI Mysore (Food and related pesticides); IICT-Hyderabad (Fine chemicals and pesticides); IIP-Dehradun (Petroleum & engine exhaust gas emissions) and CDRI-Lucknow (clinical, bio and drugs), the efforts in 11<sup>th</sup> five year plan are being made. The traceability of measurements carried out in these lead laboratories/ institutes, spread all over the country, and improvement in the uncertainty for various parameters through MiC will be established to realize the, amount of substance 'mol' and the customer satisfaction for various MiC products like CRMs.

With efforts under Indian MiC and related work being carried out at NPL & partner CSIR laboratories it is aimed to establish the equivalence of the Indian national standards with the international standards for SI-Mole and get maximum possible number of entries in the key comparison data base (KCDB) being developed at the International Bureau of Weights and Measures (BIPM), Paris. This would mean that calibration certificates issued by NPL and other Indian laboratories, which are traceable to NPL, would be acceptable globally. Industrial and trade sectors will be provided with globally acceptable quality management infrastructure at much lower cost in the country itself. In the absence of MiC & related CRMs, the Indian & other stakeholders, laboratories and industries in various areas of MiC will have to get the MiC service done outside India which will not only be costlier but also extremely inconvenient and time consuming. In addition, if the country has to face technical barrier to trade, the loss to the country will go up many fold. Trace gases & aerosol accurate and precise measurements in the environment are important and therefore should be traceable to NMIs for data QA/ QC and reliability. The above issues & perspectives of Indian NMI efforts are presented and discussed in details.