Physisorption of gases, with special reference to the evaluation of surface area and pore size distribution (IUPAC Technical Report)

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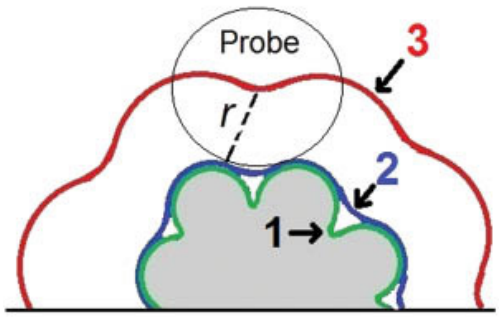
Gas adsorption is an important tool for the characterisation of porous solids and fine powders. Major advances in recent years have made it necessary to update the 1985 IUPAC manual on Reporting Physisorption Data for Gas/Solid Systems. The aims of the present document are to clarify and standardise the presentation, nomenclature, and methodology associated with the application of physisorption for surface area assessment and pore size analysis and to draw attention to remaining problems in the interpretation of physisorption data.



*Schematic representation of several possible surfaces of an adsorbent. 1: van der Waals; 2: Connolly, Probe-accessible; 3: Accessible, r-distance. (*vide supra *page 1054)*

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International Vocabulary of Metrology

An abridged version of the International Vocabulary of Metrology—Basic and general concepts and associated terms (VIM) (JCGM 200:2012, 3rd edition) (or VIM3), supplemented by annotations for some of the entries, was released in September 2015 by BIPM, the Bureau International des Poids et Mesures. The online document produced by Working Group 2 of the Joint Committee for Guides in Metrology (JCGM/WG 2) has the following features:

- all definitions, notes, and examples of the VIM3 are taken without modification from the VIM3 itself;
- the VIM3 Foreword, Introduction, Conventions, Scope, Annex, Bibliography, and List of acronyms are omitted;
- an Alphabetical index is included;
- in definitions, notes, and examples, terms designating concepts defined in the VIM3 are hyperlinked;
- some annotations are included, aimed at further clarification or comment on specific definitions, notes, or examples. The JCGM decided that the annotations are informative and not normative. They are exclusively developed by JCGM/WG2, according to procedures agreed by the JCGM

The original VIM3 can be downloaded freely as one pdf from the BIPM site. For an outline/presentation of the VIM3 release, see *Chem. Int.* May-June 2012, p. 26.

www.bipm.org/en/publications/guides/vim.html

Seminal InChI Publications

Many InChIs and quite some feat—that is the greeting offered to all interested in the IUPAC International Chemical Identifier, InChI, in a review published by Wendy Warr in *J Comput Aided Mol Des* (August 2015, 29:8, pp. 681-694; http://dx.doi.org/10.1007/s10822-015-9854-3). The article details not only the history of the project, but also its recent and current development, and celebrates 15 years of work since the project was first launched in 2000. The 14-page paper includes 275 references.

Warr recalls that, back in 2000, the increasing complexity of molecular structures made conventional naming procedures inconvenient, and there was no suitable, openly available electronic format for linking chemical structures over the Internet. InChI was developed as a freely available, non-proprietary identifier for chemical substances that can be used in printed and electronic data sources, thus enabling easier linking of data compilations and unambiguous identification of chemical substances. InChI was developed under the auspices of IUPAC, with principal contributions from the US National Institute of Standards and Technology (NIST), and more recently, the InChI Trust. While the IUPAC InChI SubCommittee has the responsibility for

continued authentication of the InChI standard, the InChI Trust, in turn, develops and supports the non-proprietary InChI standard and promotes its use to the scientific community. Version 1 was launched in 2005 and the current version (1.04) was released in September 2011. CI readers have been regularly updated on InChI, its developments and applications (A. McNaught, *Chem Int* 28(6):12-14 (2006); J. Frey, *Chem Int* 28(6):14-15 (2006); S. Heller and A. McNaught, *Chem Int* 31(1):7-9 (2009); A. Yerin, et al, *Chem Int* 35(6):12-15 (2013)).

A second article released slightly earlier, in May 2015, by the core project task group, documents the design, layout, and algorithms of InChI, and was published in *Journal of Cheminformatics* (Heller et al. (2015) 7:23; http://dx.doi.org/10.1186/s13321-015-0068-4). This 34-page article is intended to provide a reasonably detailed description without being overlong for a journal article. For a more technical description, the reader is referred to the InChI Technical Manual and the free source code of the InChI software, available from the InChI Trust website at www.inchi-trust.org .

In her conclusion, Warr reminds us that establishing a standard is not a quick process; and that we should be impressed with what InChI has achieved over 15 years. She also declares that the InChI Trust does not intend to stop there. A new application programming interface (API) is being tested. Currently, the InChI

A 4-part video, 1. What on Earth is InChI? 2. The Birth of the InChI, 3. The Googlable InChIKey, and 4. InChI and the Islands, is easily accessible @ www.inchi-trust.org

algorithm can handle neutral and ionic organic molecules, radicals, and some inorganic, organometallic, and coordination compounds. Steps to expand it to handle more complex chemical structures are underway. Work continues on polymers and mixtures. Efforts on generic ("Markush") structures are planned once funding is secured. In the longer term, consideration will be given to the InChI resolver, QR codes for InChI, macromolecules, positional isomers, crystal structures, and to extending the coverage of inorganic, organometallic and coordination compounds.

Volunteers willing to join the team will define the InChIs of the future. IUPAC and the InChI Trust continue to seek new members and people willing to help maintain and enhance the InChI standard.

For more information, contact Steven Heller <steve@hellers.com>

www.iupac.org/body/802

IUPAC Provisional Recommendations

Provisional Recommendations are drafts of IUPAC recommendations on terminology, nomenclature, and symbols, made widely available to allow interested parties to comment before the recommendations are finally revised and published in IUPAC's journal *Pure and Applied Chemistry*. Full text is available online.

Glossary of Terms Used in Extraction

Approaches for analytical-scale extraction are developing rapidly as new strategies are implemented to improve sample throughput, minimize material use in laboratory methods, and develop on-site capabilities. In this contribution, definitions and recommendations for symbols for the terms used in analytical extractions are presented. Exhaustive, microextraction, elevated temperature, microwave- and ultrasound-assisted, parallel batch, flow through systems, and membrane extraction approaches are discussed. An associated tutorial titled "Extraction" provides a detailed introduction to the topic.

Comments by **31 January 2016**

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www.iupac.org/project/2011-063-1-500