IUPAC: the role of international organisations in nomenclature and terminology in the internet age

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Chemistry, University of Southampton

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IUPAC Committee on Publications and Cheminformatics Data Standards (CPCDS).

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Robert A. Heinlein, “Where to?” 1950

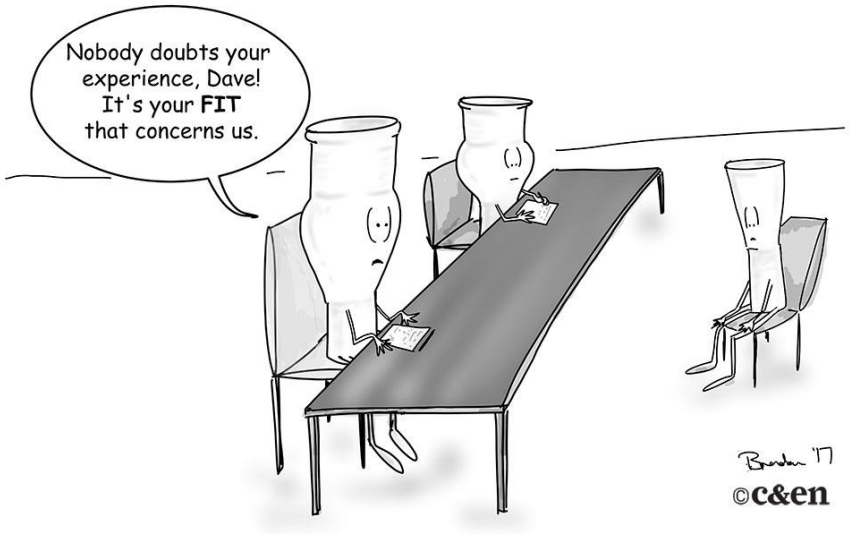
- Chemistry is not a discipline today; it is a jungle.
- We know that chemical behavior depends on the number of orbital electrons in an atom and that physical and chemical properties follow the pattern called the Periodic Table.
- We don't know much else, save by cut-and-try, despite the great size and importance of the chemical industry.
- When chemistry becomes a discipline, mathematical chemists will design new materials, predict their properties, and tell engineers how to make them — without ever entering a laboratory.
- We've got a long way to go on that one!

IUPAC & Standards

- Setting standards is at the heart of international exchange of information and trade
- IUPAC's work in establishing Chemical Nomenclature and following this with work on terminology has been critical for international collaboration both within chemistry and to other areas,
- This has often been driven by developments in chemical structures (novel structures, new characterisation methods).
- Currently contributing to an international effort coordinated by CODATA to work across the scientific disciplines to facilitate the exchange of data, driven by global humanitarian goals.

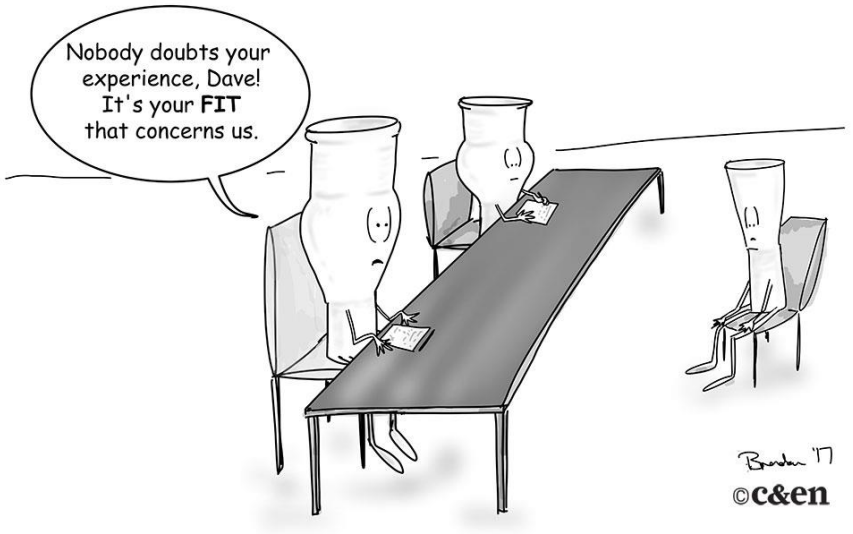
IUPAC Committee on Publications and Cheminformatics Data Standards

- IUPAC Colour* Books set out the agreed standards for nomenclature, symbols and terminology to facilitate accurate and efficient communication of chemistry.
- **Color* Books**
  - The IUPAC Color Books are the world's authoritative resource for chemical nomenclature, terminology, and symbols. Terminology definitions published by IUPAC are drafted by international committees of experts in the appropriate chemistry sub-disciplines, and ratified by IUPAC's Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS).



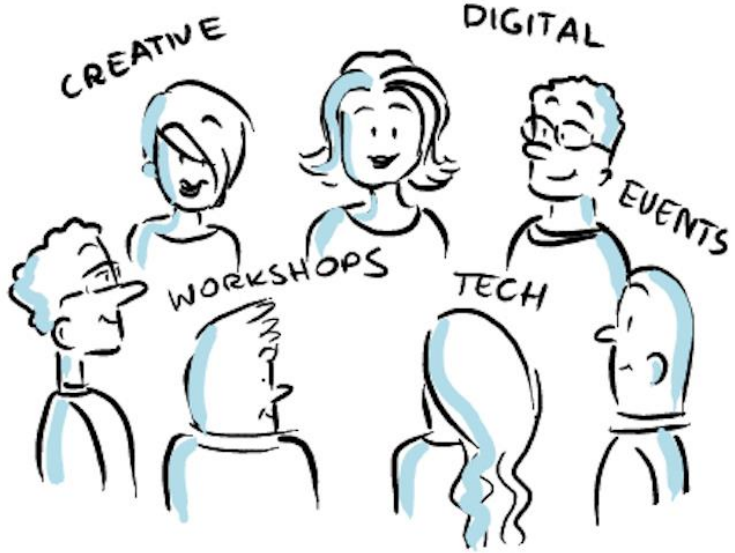
IUPAC Committee on Publications and Cheminformatics Data Standards

- Theses standards have always been needed to bridge Pure and Applied areas of chemistry, and increasingly we recognize the need to work with other disciplines.
- In recognition of the importance of DATA the remit of a key IUPAC committee was enhanced and re-directed towards the main issues of the digital age
- This resulted in The Committee on Publications and Cheminformatics Data Standards (CPCDS).



Research Data, Big Data & Chemistry

- Computational Chemistry has been a major driving force for wider computer processable chemical data (drug and materials design).
- Recognition of the massive scale of the revolution brought by automation, digital, and the potential of the resulting chemistry to impact on all the major global concerns.
- See “Research Data, Big Data & Chemistry”, in the current issue of *Chemistry International*, 39, 2017.
  - https://www.degruyter.com/view/j/ci.2017.39.issue-3/issue-files/ci.2017.39.issue-3.xml



The Internet and the World Wide Web

- The rise of the World Wide Web is radically changing the way in which chemical concepts are conveyed
- discipline specific international organisation are struggling to maintain their role in setting standards,
- It is essential that they find their place in the Web World to ensure that the knowledge (and Data) that is currently communicated on paper can be readily and accurately communicated in the digital world.

International Chemical Identifier (InChI)

- A major example of the coordination between the chemical and computer worlds
- A unique computable chemical identifier for structures
- More on this in later talks…

Energy Landscapes

- In a unique relation, each local minimum of the energy landscape corresponds to a compound capable of existence, and conversely every synthesized or realizable chemical compound is associated with such a minimum.
- According to our view, working in the field of synthetic chemistry is equivalent to exploring the landscape of free enthalpy *[sic energy?]*.
- Owing to the equivalence mentioned above of compounds capable of existence with well-defined, predetermined, locally ergodic regions on the energy landscape of chemical systems, there is no room for either the free or the arbitrary shaping of compositions and/or topologies of chemical systems by human efforts.
- **Thus, “design” is not possible, and “humans are the explorers, and not the creators of chemical worlds”**

Chemistry & Design

"Design" in Chemical Synthesis—An Illusion?**

Martin Jansen and J. Christian Schön*

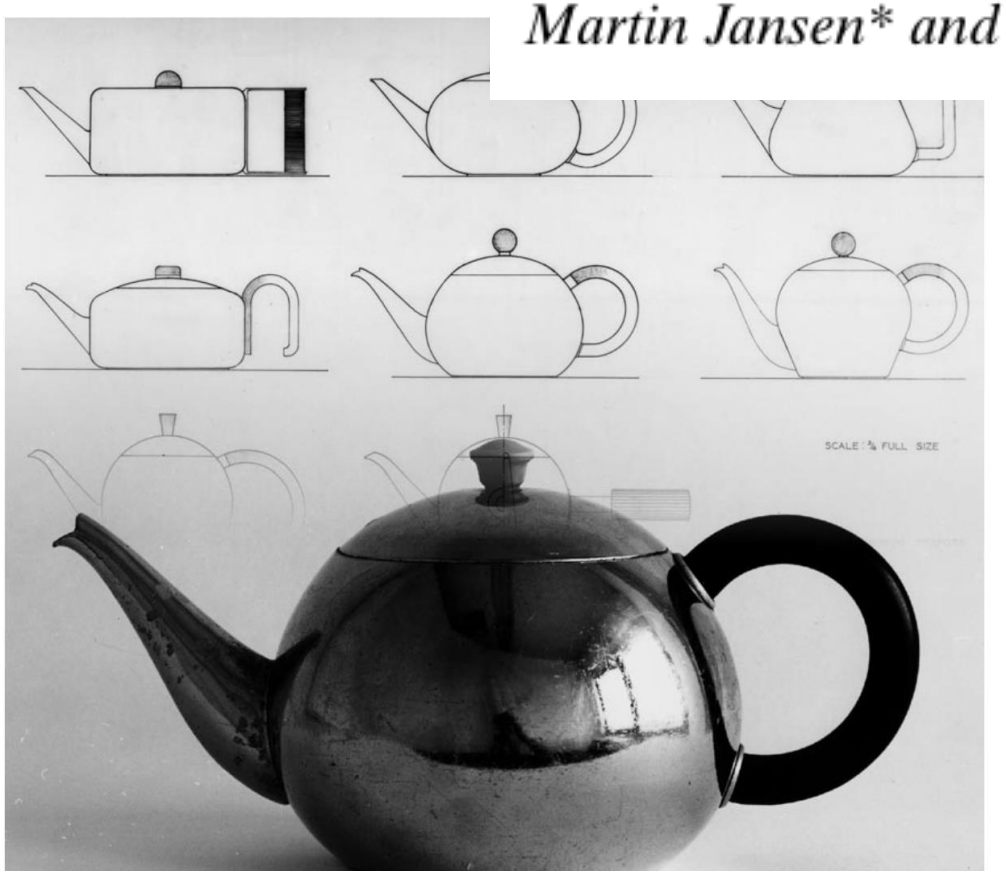


Figure 1. Teapot designs by Walter Gropius for Aluminium Ltd., London, 1935 (background) and the only type of teapot made based on these designs. *Bauhaus-Archiv Berlin.*

the Smart Tea Project

"I can go anywhere and its, like, this is me and my data. Its all there, bang."

- Chris,
a real chemist, on using Smart Tea instead of a paper lab book.

Smart Tea is about improving the information environment for chemists doing chemistry - within and beyond the lab. Smart Tea is about supporting chemists in the preparation, execution, analysis and dissemination of their experimental work.

Background

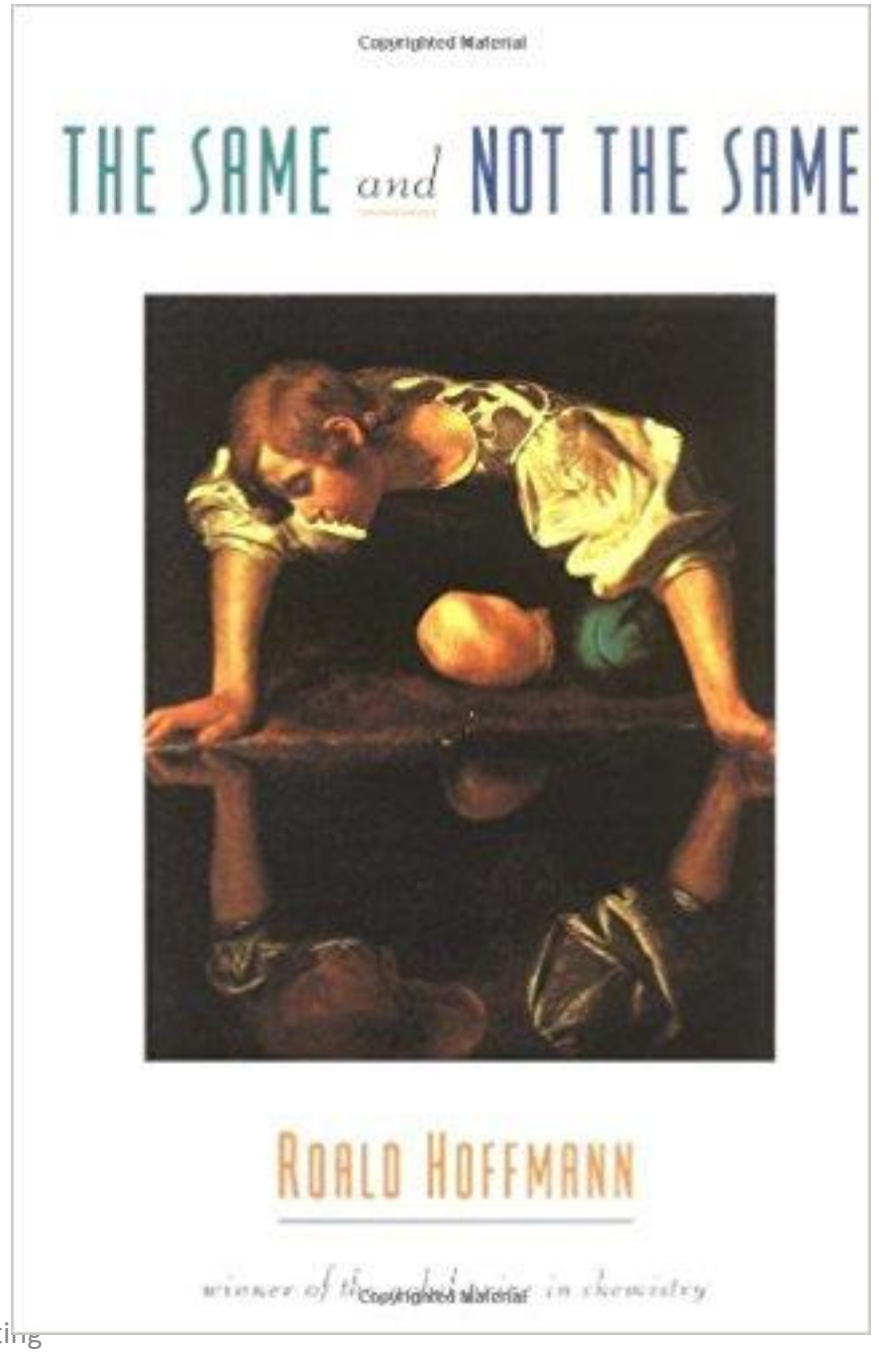
When chemists run experiments, they create a great deal of information: they describe hypotheses; they delineate methods for testing those hypotheses; they reference others' efforts in similar experiments; they record exact amounts of chemicals used, and the methods for combining them; they analyse the success or failure of these results.

For all its technical sophistication, the modern lab experiment is still recorded using the same tools as scientists have been using over the past 200 years: a bound paper lab book (pictured right).

The flexibility of the lab book makes it great for chemists while carrying out an experiment: they can move it easily from their desk to the lab bench to a shelf. The book itself, however, is a poor mechanism for making the information stored in that book available to other scientists within the lab, or for that matter, to the same scientist after the experiment has been completed: if the scientist does not have the lab book to hand, the information is unavailable.

World Wide Web

- Why do we find our selves in conflict with the W3C standards
- Same or Not the Same
- “Facts” are not always completely correct.



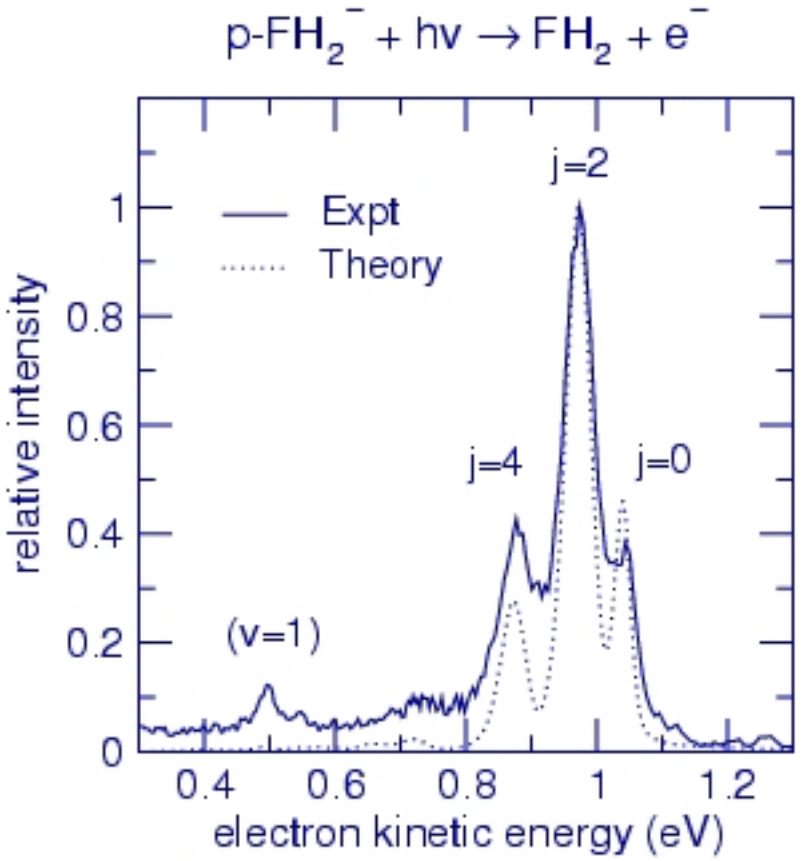
Why do we need a name?

- A convenient way to locate a position on the chemical energy landscape.
- But we only know a few details of the chemical landscape
- Other ways to do this
  - A map – simply exchange a diagram?
  - GPS
  - What Three Words
    - Retain.mostly.stage

what3words
addressing the world

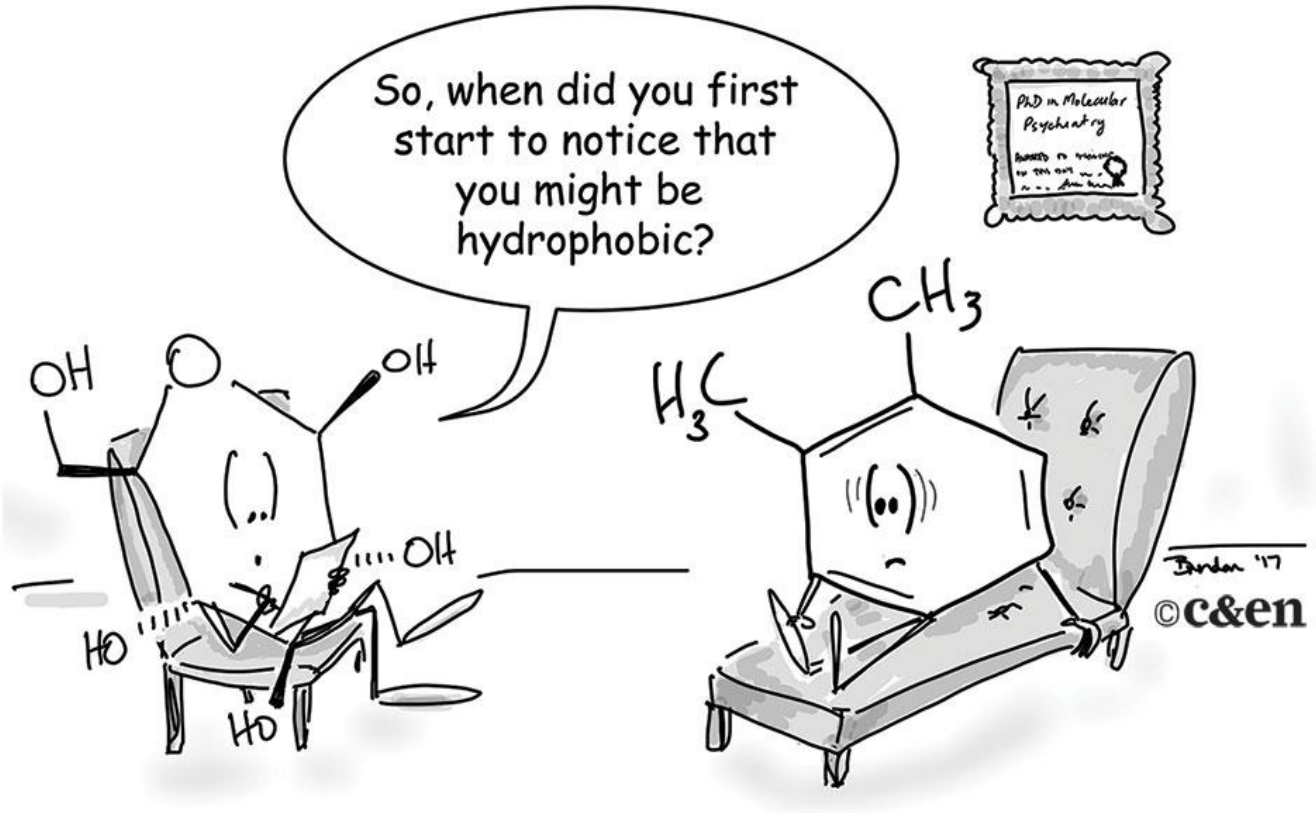
What is a structure? What is the same thing?

- What is a structure?
- What size scale?
- Key seems to be how fast or easily converted?
  - Permutation Inversion Group
- Transition States
  - These can now be observed.
  - Should we be able to give these structures names?



Before & Beyond the bond…

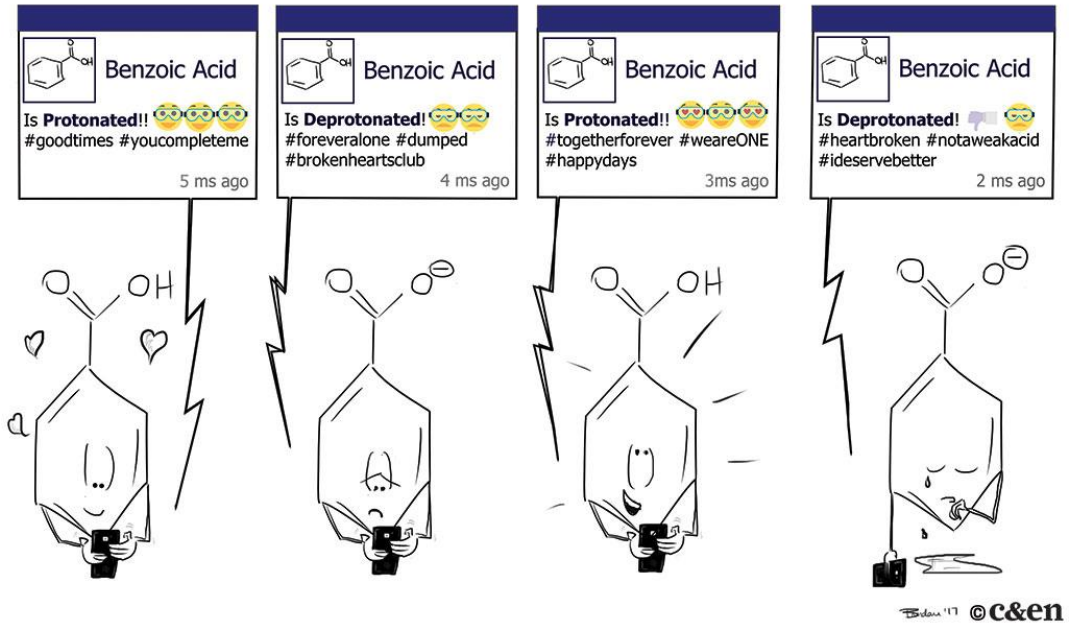
- Names based on Function
- Names based on Process
- Names based on Structure
- Names based on Bonding
- Atoms in molecules
  - Additive properties
  - Functional groups



Before & Beyond the bond…

- **Interaction with other disciplines**
- **Highlight just a few….**

- Biological – CHEBI
- Medical - WHO drug names
- Materials - nanoparticles

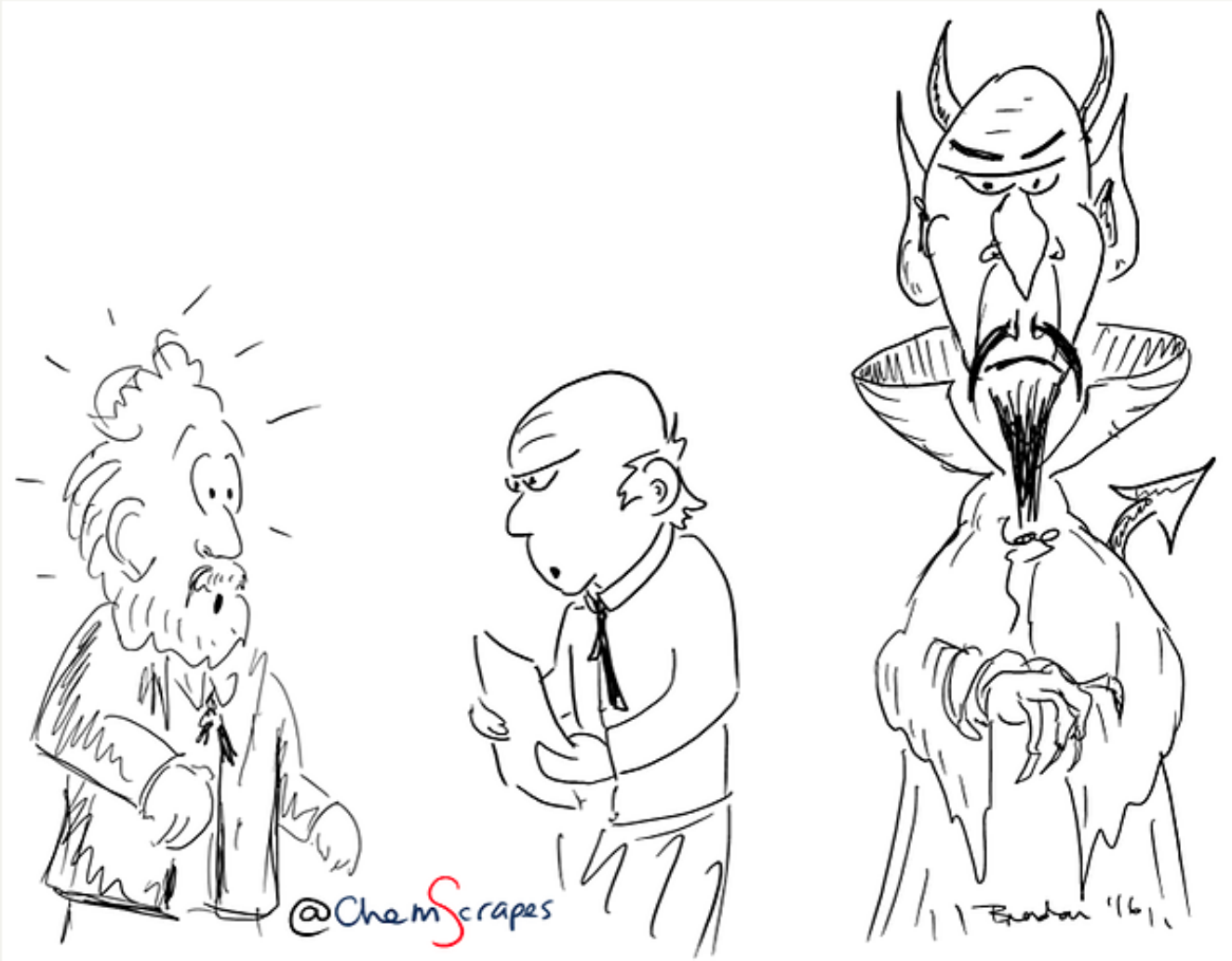


Chemistry is a Social Machine

- The aim is for the IUPAC standards to facilitate the smooth interaction of people, computers and equipment on a global scale.
- Producers and Consumers of data must not be like the non-communicating paths of a double spiral staircase (DNA)

University of Reading, Department of Chemistry

Significant moments in the history of chemistry: 1885 - Raphael Dubois coins the names Luciferase and Luciferin to describe the enzyme/molecule system responsible for bioluminescence observed in the South American Firefly, and becomes the first trademark infringement case in chemistry.



- "That's right Sir! My Client is suing you for unauthorised use of his name which he registered as a trademark in the time of King James"