

Committee on Publications and Cheminformatics Data Standards



INTERNATIONAL UNION OF
PURE AND APPLIED CHEMISTRY

CPCDS Shorts

August 4, 2020 Update

What is this?

This is the first of planned periodic updates from the IUPAC Committee on Publications and Chemical Data Standards (CPCDS) for IUPAC Bureau Members. It is not intended to be exhaustive, but rather useful and actionable. We intend to highlight a few items that you and your community should be aware of or where your action is desired. If there are items you would wish we covered in the future, please write to Leah McEwen at lm1@cornell.edu.

Calling all Experts: As you know, *Pure and Applied Chemistry* (PAC) is the IUPAC flagship scientific publication. It behooves all of us to support quality submissions. To that end, we need more expert reviewers. If you are willing to occasionally review a paper relevant to your expertise please send your name, email address, institution, and IUPAC Division/Committee affiliation to PAC@deGruyter.com. Or if you prefer, send the information to Fabienne Meyers and she will handle it.

New Taskforce on IP: IUPAC is fortunate to have so many volunteers dedicated to creating valuable resources for the wider scientific chemistry community, from editing books, to creating databases, to establishing community standards. To make sure that IUPAC protects your work, CPCDS have established a task force to work with the Secretariat to understand the various types of valuable assets IUPAC volunteers are creating, and review how they should be best protected for posterity. As the team gets underway, we will continue to provide explanations and updates through these CPCDS Shorts in the future.

CPCDS is here to help you with project data dissemination: Digital technologies enable us to measure, describe, and model phenomena much more comprehensively than ever before. However, they depend on quality data that are consistently and accurately represented. As dissemination channels for chemical data are shifting from traditional printed articles towards online data repositories, it is crucial that IUPAC data, particularly high value critically evaluated data, be accessible both to humans and machines, to support global scientific exchange. How each Division prepares its data for digital dissemination has broad implications across the entire IUPAC enterprise, from how we communicate key concepts to how we ensure authoritative IUPAC provenance. When establishing new projects, please remember you can leverage the expertise of CPCDS team to help you identify and address these complex digital data considerations.

Supporting the FAIR Data Principles for the wider Chemistry enterprise: The ability to find, access and use quality data that is interoperable across many systems and organizations worldwide is crucial for tackling international challenges such as the COVID-19 pandemic. The CPCDS Taskforce on FAIR Chemical Data has identified several emerging themes pivotal to IUPAC's position to support global access to quality chemical data, including:

- The importance of reproducibility of chemistry and the relevance of IUPAC's activities to this
- The importance of establishing trust in the chemical sciences across sectors
- The need for domain-specific repositories that ensure long term stewardship of chemistry data
- The opportunity for IUPAC to help catalyse improvements in the publication of data
- The unique position of IUPAC as a bridge between academia and industry

The Taskforce believes there is an opportunity for IUPAC to make a high level statement that highlights the importance of the FAIR Data Principles to the wider chemistry enterprise. Its aim for the second half of 2020 will be to explore recommendations for how IUPAC might arrive at such a statement. It will also reflect on the extent to which existing IUPAC standards, terminologies, guidelines and other outputs can already be used to support implementation of the FAIR principles by scientists in chemistry and other disciplines.

IUPAC to highlight innovation in data and standards at the quinquennial Pacificchem event, now scheduled for 2021: Pacificchem is the International Chemical Congress of the Pacific Basin Chemical Societies. CPCDS successfully recruited international speakers across chemistry sectors and beyond to participate in a two-day symposium highlighting "Chemistry on the Global Stage: Data, Standards, Infrastructure, and Challenges for the Future." This unique conference venue has been rescheduled for December 2021 and all speakers have indicated their desire to participate pending resolution of the pandemic.