Division V – Report to the Science Board and to Council 2025

Part 1: Summary

Division V welcomed new members at the beginning of 2024, with several additions including past young observers. The Division aims to maintain high geographic and gender diversity with now 60% female representation on the Committee. Two virtual meetings of the Committee were held in 2024, with another planned for January 2025. Past Young Observers and the Chair of IYCN are invited to all meetings, and participation is actively encouraged through, for example, the formation of small Sub Groups. Most notably a Working Group has been established to support the World Congress lecture sessions on Analytical and Forensic Science, and several members of this Working Group have agreed to provide Keynote Lectures at the July event in Malaysia.

The Division continues to contribute strongly to IUPAC outputs through the project system. In 2024, 4 projects were completed, 30 remained on-going and outputs included 4 publications since September 2023. Of the 30 active projects, 3 are very close to completion with papers now submitted to PAC for review, and 19 relate to the work of the Division's two main Sub-Committees: Metrology in Chemistry (SMiC); and Solubility and Equilibrium Data (SSED). Of the remaining projects, 2 are aligned with IUPAC's Gold Book update, 5 are considering terminology and guideline requirements for emerging technology, 2 cover education and outreach and 1 relates specially to Green Chemistry. As such, the Division considers that its work is fully aligned with IUPAC's Vision, including the drive for the adoption of FAIR principles. Of note to the Digital Agenda, CPCDS were involved in preparing the final output of the critical compilation of acid pKa values in polar aprotic solvents, and the Division leads on a project to provide guidance for the compilation, critical evaluation and dissemination of chemical data. A key objective of the Division will be to ensure that FAIR principles are imbedded in all future project work, and while only 1 new project was approved in 2024 (submissions impacted by budgetary concerns) at least 3 are currently in various stages of planning. One of these will involve multiple other Divisions within IUPAC, and this is an important theme, with many of the active projects involving interactions with, for example, Divisions II, VI, CCE and CPCDS

As part of its outreach and the promotion of its disciplines, the biannual awards organized by the Division continue to be an important part of on-going activity. Plans are now well advanced for the Analytical Chemistry Medal (lifetime achievements) and the Young Innovator Award (promising emerging investigator) which will be presented during the Biennium meeting in Kuala Lumpur in July. In addition, the Franzosini Prize and Balarew Award were given this year at the 21st International Symposium on Solubility Phenomena and Related Equilibrium Processes (ISSP) which took place from September 9-13, 2024, in Novi Sad, Serbia. The ISSP is an important event in the calendar of the SSED, with over 60 participants attending the conference from 17 countries.

Part 2: Plans and Priorities

Division V is looking forward to working with the Science Board to implement IUPAC's strategy and to respond to any proposed structural reorganizations. Measurement is central to all disciplines of chemistry and to emerging fields of science and we will seek to expand and retain our volunteer base to enable its effective deployment to areas of priority.

In the meantime, the Division will continue to deliver and propose new project areas in-line with IUPAC's Vision. Emphasis will be on:

- Completing projects that have been running for more than 5 years by encouraging activity and offering Committee support to strengthen the associated expert teams,
- Contributing actively to the update of the Gold Book,
- Delivering outputs from our two main Sub-Committees (SMiC & SSED),
- Ensuring publications conform to FAIR principles, and involving CPCDS more actively in future project proposals and delivery,
- Encouraging ideas from new technology areas and from emerging professionals using our committee networks.

Outreach, engagement and dissemination will continue to feature highly in our agenda for the next two years. Traditionally this has been achieved by involvement of Division V in the committee work of other organizations, such as ISO, BIPM, CITAC and CODATA. While this committee representation will continue, we will seek to extend this by greater use of social media and a working group of committee members will be created specifically for this purpose. We will also seek to enhance the profile of the Division by more active promotion and seeking potential sponsorship of our biannual awards.

Finally, building a vibrant community of contributors will be a specific area of focus over the coming years. Efforts in this respect are on-going, with an increasing number of individuals now invited to the Division's on-line meetings. We will augment these efforts by:

- Increasing our engagement with IYCN,
- Increasing our number of working groups to ensure all committee members are involved in some Divisional activity,
- Retaining regular contact with past committee members, those proposed (but not successful) for election, and all YOs that attend our meetings,
- Ensuring active representative from the Division Committee on all IUPAC Standing Committees.

Part 3: Key Activities and Achievements 2024/25

(a) Global scientific cooperation and collaboration that creates a common language of chemistry, including data or technical standards, nomenclature, terminology, and symbols;

The Division has two very active Sub-Committees that are responsible for significant technical output in standards, nomenclature, critical data, terminology and symbols

The Sub-Committee on Metrology in Chemistry (SMiC) stems from earlier efforts in quality assurance and has evolved to address measurement uncertainty, human errors, and metrological education. Two current major project streams are in error analysis and metrology guides with seven active projects addressing these areas

The Sub-Committee on Solubility and Equilibrium Data (SSED) originates from the 1970's and collaborates with organizations like NIST. SSED encourages task groups for data evaluation and compilation projects. Its achievements include publishing volumes of the Solubility Data Series, maintaining the IUPAC Stability Constants Database, and launching databases for ionic liquids and thermodynamic data. SSED currently has twelve active projects, some of which are now close to completion.

There are thirty active projects running within the Division, and four that were concluded over the course of 2024. Many of these projects involve cooperation with other Divisions and Standing Committees. Although over 50% of projects are associated with the Divisions' two Sub-Committees there are other important areas of focus:

- Having recently completed an update of the Orange Book, the Division is looking forward to uploading and amending terms for inclusion in IUPAC's updated Gold Book. This process should be possible without major re-writing and publishing of new recommendations, and the associated projects await decisions on how best to proceed with this work,
- The Division recognizes the importance of establishing nomenclature, terms and symbols in emerging areas of science and has five related active projects, including one on Wearable Devices which featured as one of IUPAC's Top Ten Technologies in 2023,
- Adopting FAIR principles is now essential in all the Divisions' outputs. In this regard, the Division leads a project to provide guidance for the compilation, critical evaluation and dissemination of chemical data.

(b) Interaction with chemistry organisations, professional societies, industry and other relevant bodies to facilitate best practice in chemistry and chemistry education, or which support educational initiatives in data standards and management;

Because the focus of Div V includes all aspects of the chemical measurement process, its joint activities are extensive and include:

- Providing validation guidelines for LC-MS with Div VI and Div VII,
- Aspects of isotope ratio measurements with Div II,

- Development of guidance for evaluation of chemical data with Div I, Div II, Div IV, and CPCDS.

This cross disciplinary effort will be an increased feature of the work of the Division through the course of the current Biennium, with a further priority to ensure increased activity in its larger projects, and in those that have been active for more than 5 years. Of note is the largest project in the Division which is reviewing best practice in the education of analytical chemistry, and which delivered its first output publication in 2024 (reference 8 in Part 4).

The Division also has representation on external working groups and committees. Most notably, the SMiC liaises with key international bodies such as the Joint Committee for Guides on Metrology (JCGM), focusing on developing standards like the Guide to the Expression of Uncertainty in Measurement. Members of the SMiC have communicated via email during 2024 to discuss several draft documentary standards and guidelines.

(c) Connections with cognate disciplines and educational communities, including outreach or engagement initiatives and those that contribute to sustainable development;

The Division contributes to relevant international meetings as part of the dissemination of its project outputs. Most notable in this regard is that the SSED organizes the International Symposium on Solubility Phenomena. The 21st event in this series took place from September 9-13, 2024, in Novi Sad, Serbia. The two awards that are managed by the SSED were both presented at the Symposium. The Paolo Franzosini Prizes for career recognition were given to Cezary Gumiński and Christian Ekberg; and Märt Lõkov received the inaugural Christo Balarew Award for young scientists. This Symposium was attended by more than sixty registered participants from seventeen countries worldwide. The invited speakers delivered five plenary and eight keynote talks.

As part of its outreach and desire to promote the discipline of Analytical Chemistry, The Division instituted two biannual Awards in 2021: the Analytical Chemistry Medal for lifetime achievements; and, the Young Innovator Award recognizing promising emerging investigators. Plans are well advanced for the third set of Awards which will be presented during the Biennium meeting in Kuala Lumpur in July. A call for nominations was sent out and distributed through multiple channels in July 2024, with nominations received from September through to the end of December. An Awards Committee has been formed to review all nominations and announcements are planned for early in 2025.

(d) Promotion of diversity and inclusiveness in the profession of chemistry, or of values and ethics in science through responsible practice.

The Division aims to maintain high geographic and gender diversity. The Division Committee for 2024/25 includes several new members and some past young observers. Representation now covers North and South America, Asia, Europe, Africa and Oceania, with a 60:40 female: male balance. Two virtual meetings of the Committee were held in 2024, with another planned for January 2025. Past Young Observers and the incoming Chair of IYCN are invited to all meetings, and participation is actively encouraged. The virtual meetings act as a mechanism for updating and educating the Committee on IUPAC, and to discuss projects and other upcoming

events. Two small Sub-Groups were formed to consider participation in a virtual General Assembly (should this be held) and to support the World Congress lecture sessions on Analytical and Forensic Science: a further will soon be initiated to consider options for outreach through social media channels. The Sub-Groups have proved useful in getting Committee involvement and interaction and will be a continued theme for 2025.

The Division now has full representation on all IUPAC Standing Committees and aims to actively contribute to associated goals. This includes new representation on the Interdivisional Committee on Green Chemistry for Sustainable Development and the Committee on Ethics, Diversity and Inclusion. Regarding Sustainable Chemistry, the Division leads in an important project on Green Analytical Chemistry, with the current focus being on the solvent heavy area of sample preparation.

Part 4: Tables

Projects

A list of projects is provided below. End dates are currently under review as part of the Divisions annual cycle of update and discussion with project leads.

On-going			
Project Numbers	**Lead**		**Planned End Date**
2009-006-1-500	Ellison	Experimental Requirements for Single-Laboratory Validation	31/12/2024
2013-034-1-500	Gadzuric	Mutual Solubility of Rare Earth Metal (Sc, Y, Lanthanides) Bromides in Molten Alkali Bromides	31/12/2024
2015-008-2-500	Apak	Critical Evaluation and Vocabulary of Chemo-sensing and Determination Methods for Explosive Residues On-Site and in the Field	31/12/2024
2015-020-2-500	Leito	Critical compilation of acid pKa values in polar aprotic solvents	31/12/2025
2015-024-2-500	Hibbert	Metrology and Measurement Uncertainty Brochure	31/12/2024
2015-044-2-500	Bendova	Critical evaluation of data on solubility and liquid-liquid equilibria in binary mixtures of 1-alkyl-3-methylimidazolium based ionic liquid and molecular solvent	31/12/2025
2016-005-1-500	Nordstrom	Calcium sulfate in water	31/12/2023
2017-022-1-500	Oracz	Mutual Solubility Halogenated Aliphatic Hydrocarbons C1-C14 with Water	31/12/2025
2017-025-1-500	Eysseltova	Solubility in Systems with Potassium Nitrate (Part 3 of Volume 89 of the Solubility Data Series)	31/12/2025
2018-009-2-500	Shaw	Guidance for the Compilation, Critical Evaluation and Dissemination of Chemical Data	31/12/2025
2018-010-2-500	Flores	Microwave Induced Combustion (Critical Evaluation and New Applications)	31/12/2024
2018-025-1-500	Filella	Critical evaluation of homogeneous equilibrium and solubility constants of gadolinium in environmental and biological-relevant conditions	31/12/2024
2019-012-1-500	Kuselman	Influence of a mass balance constraint on uncertainty of test results of a substance or material and risks in its conformity assessment	31/12/2024
2019-028-1-500	Hefter	Critical Evaluation of Metal-Sulfate Equilibrium Data	31/12/2025
2019-039-3-500	Mester	A review of current status of analytical chemistry education	31/12/2025
2020-025-2-500	Carvalho	Solubility of CO_2 in glycols and glycol ethers	31/12/2025
2021-011-1-500	Magalhaes	Gold Book update of terms from the Glossary of Terms Related to Solubility	30/06/2024
2021-015-2-500	Psillakis	Greenness of official standard sample preparation methods	31/12/2024
2021-017-2-500	Kuselman	Harmonization of approaches to interlaboratory comparison of qualitative and related property values of a substance or material	31/12/2025
2021-018-1-500	Mester	Gold Book Update of Terms for Analytical Chemistry	31/12/2025
2021-023-1-500	Acree	Solubility of Benzoic Acid and Substituted Benzoic Acids in Both Neat Organic Solvents and Organic Solvent Mixtures (Supplement to Solubility Data Series Volume 99)	31/12/2024

2021-036-1-500	Piscitelli	LC-MS quantitative method validation and performance: an exemplified guide	31/12/2024
2022-002-2-500	Pinho	Assessment of Reliability and Uncertainty of Solubility Data	31/12/2024
2022-008-4-500	Minguzzi	Introducing the IUPAC Seal of Approval for a wider adoption of IUPAC recommended symbols, terminology and nomenclature: Stage 1 - Symbols	31/12/2024
2022-031-1-500	Guminski	Rare Earth Metal Sulfates in Water and Aqueous Systems (SDS series)	31/12/2026
2023-006-1-500	Torsi	Assessing the need for terminology, standards and guidelines for wearable devices that provide chemical / biochemical measurement readouts	31/03/2025
2023-010-2-500	Labuda	Electroanalytical flow through systems for monitoring of biologically active species	31/12/2025
2023-016-1-500	Kuselman	IUPAC/CITAC Guide for interlaboratory comparison of nominal (qualitative) and ordinal (semi-quantitative) characteristics of a substance or material	31/12/2025
2023-028-1-500	Hibbert	IUPAC Brief Guide to Metrological Terms in Chemistry	31/12/2025
2024-012-2-500	Kuselman	Advanced methods for assessment of risks of false decisions in analytical chemistry (testing) laboratories – basic concepts and associated terms	31/12/2026
Completed projects			
2017-005-3-500	Labuda	-	31/12/2023
2015-021-1-500	Hibbert	-	31/12/2023
2014-025-1-500	Hibbert	-	31/12/2023
2021-009-2-500	Peterson	-	31/12/2023

Publications Since the Last Council Meeting (August 2023)

1. A brief guide to measurement uncertainty (IUPAC Technical Report). A Possolo, D.B. Hibbert, J. Stohner, O. Bodnar, J.Meija, Pure Appl Chem. (2024). https://doi.org/10.1515/pac-2022-1203
2. IUPAC Technical Report: Methods for the SI-traceable value assignment of the purity of organic compounds, Steven Westwood,Katrice Lippa, Yoshitaka Shimuzu, Beatrice Lalerle, Takeshi Saito, David Duewer, Xinhua Dai, Stephen Davies, Marina Ricci, Annarita Baldan, Brian Lang, Stefan Sarge, Haifeng Wang, Ken Pratt, Ralf Josephs, Mikael Mariassy, Dietmar Pfeifer, John Warren, Wolfram Bremser, Stephen Ellison, Blaza Toman, Michael Nelson, Ting Huang, Ales Fajgelj, Ahmet Gören, Lindsey Mackay and Robert Wielgosz 2023 Pure and Applied Chemistry, https://doi.org/10.1515/pac-2020-0804.
3. A novel multisensory quality index of a food product: An analysis of a sausage properties. Chemometrics and Intelligent Laboratory System.s T.Gadrich, F.R. Pennecchi, I.Kuselman, D.B. Hibbert, A.A. Semenova, M. Salikova (2023) 237C, 104815, https://doi.org/10.1016/j.chemolab.2023.104815
4. IUPAC Technical Report: IUPAC/CITAC Guide: Evaluation of risks of false decisions in conformity assessment of a substance or material with a mass balance constraint. Pennecchi, Francesca R., Kuselman, Ilya and Hibbert, D. Brynn Pure and Applied Chemistry, (2023). https://doi.org/10.1515/pac-2022-0801
5. IUPAC-NIST Solubility Data Series Volume 105: Solubility of Solid Alkanoic Acids, Alkenoic Acids, Alkanedioic Acids and Alkenedioic Acids Dissolved in Neat Organic Solvents, Organic Solvent Mixtures, and Aqueous-Organic Solvent Mixtures. III. Alkanedioic Acids and Alkenedioic Acids, E. Acree, Jr. and W. E. Waghorne, Journal of Physical Chemistry Reference Data, 52, 033102-1 (2023) https://doi.org/10.1063/5.0147933.
6. Compendium of Terminology in Analytical Chemistry: IUPAC Orange Book. prepared for publication by D Brynn Hibbert, The Royal Society of Chemistry, 2023 [ISBN 978-1-78262-947-4]; DOI: https://doi.org/10.1039/9781788012881. The story of the 15-year, 57-contrubutor effort to produce the Orange Book.
7. Terms of Latin origin relating to sample characterization (IUPAC Technical Report). V. K. Peterson, M. Bianchini, K. W. Chapman, M. Elice, D. B. Hibbert, P. Roche, L. Silvano and L. Stievano, Pure Appl. Chem. (2024); 96(11): 1531-40 https://doi.org/10.1515/pac-2022-1103
8. Incorporation of analytical chemistry in the undergraduate curriculum: examples from different regions of the world. T. J Wenzel., P. B. C Forbes., B. C. Galarreta, B. A. Patel, M. Vogel, D. K. Y. Wong, Analytical and Bioanalytical Chemistry, 416, 3997–4006 (2024) https://doi.org/10.1007/s00216-024-05360-3

Conferences

1. 21st International Symposium on Solubility Phenomena and Related Equilibrium Processes (ISSP21), September 9-13, 2024, Novi Sad, Serbia