

## 2022 Activity Report

Inter-commission B5-B2 working group " Laboratory Astrophysics Data Compilation, Validation and Standardization: from the Laboratory to FAIR usage in the Astronomical Community ".

[https://www.iau.org/science/scientific\\_bodies/working\\_groups/335/](https://www.iau.org/science/scientific_bodies/working_groups/335/)

The overall objectives and goals of the B5-B2 working group is to provide a platform where to discuss the FAIR (Findability, Accessibility, Interoperability, Reuse) usage of laboratory astrophysics data in astronomy and astrophysics. The 3 core milestones of the working group have been for Year 1, establish an overview of the state of the art of the communities (astronomy, physics, chemistry, planetary, etc....), for Year 2) identify the bottlenecks and challenges encountered for FAIR exchange and usage of laboratory astrophysics data, and for Year 3) provide recommendations to the IAU community.

The WG group was created in November 2021 with the following members : ML Dubernet (Obs. Paris, France), B. Berriman (Caltech, USA), Farid Salama (NASA Ames, USA), Friedrich Kupka (UNIVIE, Vienna, Austria), Jiayong Zhong (Beijing Normal University, China). A new member, Randall Smith (CfA, Harvard Univ., USA), was included in 2022.

The 2022 actions of the WG were linked to the first milestone of the WG, i.e., to establishing an overview of the state of the art for the involved communities. The 2022 activities led to one contributed and 2 invited presentations in conferences (ICAMDATA/Sept, IAU 371 Symposium/August, SPIG2022/Sept), to 5 seminars at institutes (in France/April and in Korea /January, July, August), to presentations to the IUPAC (July), to the IVOA (April), to the VAMDC Annual Meeting and to its Board of Directors (June) and to 3 refereed proceedings to be published in 2023. Through those presentations we met the objectives of connecting to various communities and to international bodies that deal with standardisation in physics/chemistry and in astronomy.

1) Study of the state of the art of practices in the database community as well as in the astrophysics community related to the tools commonly used to analyze astronomical data and to numerical codes used to model astronomical media. Two on-line surveys were designed for this purpose: A database survey (<https://forms.gle/Q9T2FqZiEdjxYGXR6>) with 20 answers provided so far and an astro Codes/Tools survey (<https://forms.gle/iAb7HYAXSeVXgkhY9>) with 8 answers provided so far in spite. In both cases, advert mails were sent via the IVOA mailing lists and other lists. The preliminary results of the surveys were presented at the WG session organised at the IAU GA in Busan, 2022 (DOI: 10.5281/zenodo.697929).

2) The WG organised a session at the IAU GA, Busan 2022 (DOI : 10.5281/zenodo.7050655) entitled "**Laboratory Astrophysics Databases: from the provider to the user: encouraging FAIRness** »

The **SOC** was composed of the WG members (ML Dubernet (CB5, CB2, CH2), B. Berriman (CB1, CB2), Farid Salama (CB5, CF3, CH2), Friedrich Kupka (CB5, CF2, CG4), Jiayong Zhong (CB2)) in addition to IAU members from a variety of commissions/divisions (Beatriz Barbuy (Division G WG Active B stars, Division J),

Masatoshi Ohishi (Advisor CF3, CB2, CB4, Division A, F, H), Miriam Rengel (VP CF2, CB5, Division B, C, E, H), Dongsu Ryu (CB1, CB5, Division D, J, inter-division B-H-J)) providing a broad representation of the IAU community and scientific bodies.

The program is provided below :

- WG Activities and Plans; FAIR in VAMDC (ML Dubernet) - **10.5281/zenodo.6979299**
  - FAIR principles in IVOA (B. Berriman) - **10.5281/zenodo.7049804**
  - The NASA Ames PAH IR Spectroscopic Database (C. Boersma) - **10.5281/zenodo.7042959**
  - Laboratory Astrophysics Databases on Grains and Ices: From the Laboratory to the Users (Cornelia Jäger) – **10.5281/zenodo.7040441**
  - About the atomic and molecular databases in the planetary community (Miriam Rengel) - **10.5281/zenodo.7040446**
  - Examples of astro analysis tools: ENIIGMA (Will Rocha) - **10.5281/zenodo.7040458**
- General Discussion and concluding remarks

A proceeding on that session will be included in the 2023 proceedings of the of “IAUS 371: Honoring Charlotte Moore Sitterly: Astronomical spectroscopy in the 21st century” held as a focus meeting at the Busan 2022 general assembly.

3) The WG contacted the VAMDC Consortium that maintains one of the major Atomic & Molecular Data e-infrastructure VAMDC (<https://vamdc.org>) and suggested to perform a FAIR analysis of the VAMDC infrastructure. Dr C.M. Zwölf (Paris Observatory, France) performed the FAIR analysis of the VAMDC using a FAIR model from RDA. This led to a contribution at the IAU GA Busan 2022, to a contributed talk at the ICAMDATA conference (<https://www.icamdata2022.it/>) and to a proceeding to be published in 2023 in EPJD Topical Issue "Atomic and Molecular Data and Their Applications: ICAMDATA 2022", as well as to a presentation at the french section of the IVOA (ASOV) in Spring 2023 (<https://asov.obspm.fr/journees-asov-2023/>)

4) A large survey on state-of-the art was presented in the Keynote Lecture “Atomic and Molecular Databases - Open Science for better science and a sustainable world » at the “IAUS 371: Honoring Charlotte Moore Sitterly: Astronomical spectroscopy in the 21st century” held as a focus meeting at the general assembly (DOI : 10.5281/zenodo.6979352). A related paper will be published in 2023 in the IAUS 371 symposium proceedings.

5) The conclusions of the first milestone were also presented at the SPIG2022 conference (<http://spig2022.ipb.ac.rs/>) “Towards a Global Network for Laboratory Astrophysics Activities and Data: Better science and a sustainable world” (DOI : 10.5281/zenodo.7070971)

6) The WG participated to a proposal (LoI 2024-2173) of a focus meeting for the next IAU GA 2024 in South Africa “IVOA Focus Session: Community Engagement and Open Science in the Virtual Observatory” with a session related to the inter-commission activities. Here ist the extract of the text :

(...) Interpretation of these new data sets will require ever refined atomic and molecular (A&M) data and the capability of the various laboratory astrophysics databases and A&M e-infrastructures such as the VAMDC that connects about 41 A&M databases. The IAU B2-B5 inter-commission working group is

currently involved in providing a state-of-the art report on the existing A&M resources and on the astrophysical numerical codes/tools that use A&M data. The working group wishes to identify the bottlenecks in providing the data to the astronomical community and in the FAIR usage of the A&M data by the astronomical community, and in fine to provide practical and political recommendations related to optimizing the process from laboratory data to astrophysics and vice-versa. The IVOA defining standards and protocols for VO interfaces, tools and astrophysical codes could encourage and develop within its standards this FAIR usage of A&M data. (...)

7) The WG interacted with the IVOA, the major international body for the standardisation of exchanges of astrophysical data, so that A&M data citation be considered in the standards of the IVOA in astro tools and numerical codes (this is an outcome of the surveys of databases providers – see section 1)

8) A Commission B5 Zenodo community has been created (cb5-labastro). It includes all activities of the B5 commission encompassing the B2-B5 WG activities. This community can be used for any purpose linked to the "Laboratory Astrophysics Data" activities : <https://zenodo.org/communities/cb5-labastro/>.