Minutes of the 1st Management Committee Meeting of the COST Action

CA18202 - Network for Equilibria and Chemical Thermodynamics Advanced Research

COST Association, Av. Louise 149, 1050 Brussels

Brussels, 2nd October 2019

ACTION Status at the MC1

- Action parties: 20 COST countries
- CSO approval: 04/06/2019
- Start date: 02/10/2019

1) Agenda and Materials

The agenda is in Annex 1. The meeting was organised following a participatory methodology. The presentations given throughout the day are in Annex 2. The supporting materials on networking tools and tasks of the Management Committee are in Annex 3 and 4.

2) Participants and Hosting Team

Mónica Pérez-Cabero (Science Officer (SO) assigned to this Action) and Carmencita Malimban (Administrative Officer assigned to this Action) hosted the meeting. Further colleagues from the COST Association supported the hosting team in the afternoon session "How to manage the COST Action".

The hosting team welcomed the participants (list in Annex 5). The participants introduced themselves and expressed their main interest for their participation in this COST Action.

3) Pre-requisites for the Decision Making

During the day, the participants acknowledged and agreed to comply with the Rules of Procedure for the Management Committee from Annex I *COST Action Management, Monitoring and Final Assessment (COST 134/14: http://www.cost.eu/download/COST_Action_Management_Monitoring_and_Final_Assessment).*

Before any decision was taken, the SO verified that the minimum of 2/3 of the parties present, the necessary quorum was achieved allowing the Management Committee meeting to officially take place in accordance with Article 9 of the Rules of Procedure for the Management Committee (see *http://www.cost.eu/download/COST_Action_Management_Monitoring_and_Final_Assessment).*

4) Relevant Information to the Management Committee

During the day, the hosting team provided the Management Committee (MC) with information on:

- The main features of the COST programme and the COST Excellence and Inclusiveness Policy.
- The COST Actions, participation in COST Actions, the networking tools and the financial rules for their implementation and the COST Grant System.
- The rules for the reimbursement of expenses for attending meetings and/or give training in training schools.
- The tasks for managing the Action.

5) Discussions on the Action Aims, Implementation and Management

a. MoU Tasks and Deliverables: Working Group Meetings + Use of the COST networking tools

After an introduction by the Main Proposer, the participants divided in Working Groups for discussing the tasks and deliverables. The results are presented below.

Following, the hosting team presented the COST Actions, the networking tools and financial rules. The participants returned to the WGs to discuss the funding of the activities needed to achieve the Action Objectives using the COST networking tools. The hosting team supported the WGs on the discussions clarifying the COST rules and giving examples of best practice. The results were used as input for the draft proposal for the Work and Budget Plan for the upcoming Grant Period discussed below in these minutes:

WG1: NECTAR for highly hydrolysable (HHC) and/or low-valence state (LVC) cations.
Reported by: Montserrat Filella (CH)
MC members preliminarily listed as members of the WG (in alphabetical order): Elvira Bura-Nakić (HR), Montserrat Filella (CH), Elżbieta Gumienna-Kontecka (PL), Petr Hermann (CZ), Olga Iranzo (FR), Přemysl Lubal (CZ), Demetrio Milea (IT), Igor Povar (MK).
Summary of the Discussion Outcomes: <u>Session 1: MoU Tasks and Deliverables</u> The members of WG1 confirm and accept the WG1 tasks and activities declared in the MoU. Moreover, we identified the following background issues: 1) This WG is supposed to work on many elements of the periodic table, probably more than half of them. They include two very different types of elements (and thus of questions to be tackled): highly hydrolysable elements and low valence state cations. This means that two different teams will be needed. WG1 leader and co-leader have expertises that allow for these two teams to be organised. 2) The media mentioned in the MoU, including geochemical and radwast, cover a huge range of conditions. Thus, the two teams above will need to consider a wide range of conditions too. On the base of the above considerations, the tasks and deliverables of this WG will be: 1 – To set up the frame of the work of the group. This means elements and conditions to be covered. 2 – How to experimentally produce reliable thermodynamic data. 2a – Identify the main experimental limitations. 2b – Establish the adequate experimental and calculation procedures. 2c – Produce final guidelines. 3 – Thermodynamic data most needed. 3a – Identify the elements and conditions more important for the action stakeholders. 3b – Critically evaluate existing data. 3c – Clearly identify the data that would be necessary to determine experimentally. 4 – Alternative methods to be used when experimental determination is not possible. 5 – Importance of the kinetics of ligand-exchange. How to identify the mechanism and how to quantify the effect, in particular in the case of association-type mechanisms.

Step 1 needs to precede 2 to 5.

Steps 2 and 3 should follow and can be done in parallel.

Steps 4 and 5 need to be considered at the end.

Session 2: Using the COST Networking tools in the next 12 - 18 months

First six months (or until the first meeting):

1) We need to have the first meeting as soon as possible. In the first meeting, we need to create the two teams and each team needs to discuss the tasks and deliverables above and distribute the work to be done for tasks 1, 2 and 3.

2) We need to create a collaborative system that simplifies the exchange of information and the achievement of the tasks. This needs to be created as soon as possible.

3) We need to identify other actors in the field. Many people in the geochemical, radwaste and environmental fields deal all the time with prone-to-hydrolysis metals. In particular, the radwaste community, works continuously with these elements. A significant part of the mining industry too. Our aim is two-fold: (i) incorporate some of them to the WG; (ii) identify and understand the needs of stakeholders concerning these elements.

WG2: NECTAR for strong and/or multifunctional ligands, macromolecules, polyelectrolytes.

Reported by: Petr Hermann (CZ)

MC members preliminarily listed as members of the WG (in alphabetical order):

Sabriye Aydinoğlu (TU), Urte Bubniene (LT), Axel Buchholz (DE), Natalia Busto (ES), Isabel Cavaco (PT), Eva Anna Enyedy (HU), Eva Freisinger (CH), Sofia Gama (FR), Slobodan Gadžurić (RS), Enrique García-España (ES), Elżbieta Gumienna-Kontecka (PL), Petr Hermann (CZ), Olga Iranzo (FR), Iwona Lakomska (PL), Andreia Leite (PT), Přemysl Lubal (CZ), Demetrio Milea (IT), Arūnas Ramanavičius (LT), M. Amélia Santos (PT), Matteo Tegoni (IT), Katalin Varnágy (HU), Emel Yildiz (TU).

Summary of the Discussion Outcomes:

Session 1: MoU Tasks and Deliverables

During the 1st MC meeting, we agreed that tasks in MoU are still valid, as given below:

1) Thermodynamic and kinetic data of complexes with potential medicinal and environmental applications.

2) New data on metallophores/siderophores and on their interaction with high-valent metal ions

3) Review/critical evaluation of data and methods/techniques used for equilibrium and kinetic studies of multifunctional ligands

4) Determination of metal-binding sites in multidentate ligands, as peptides or proteins.

5) Development of guidelines for determination of equilibrium constants in “problematic” systems.

We discussed how the tasks can be reached and which order will be suitable to follow (see below). It was said that well proven methodology is basis for determination of reliable equilibrium constants. In some systems, knowledge of kinetics is also important to get reliable equilibrium data.

Session 2: Using the COST Networking tools in the next 12 – 18 months

1) Guidelines for determination of stability constants of strong/highly stable complexes.

2) Novel ligands for possible biological/medical application will be investigated through collaborative studies.

During the discussion, it was said that it would be hard to get very conclusive data for any family of ligands during the first 12 months. We should focus on collaborative effort to define “good laboratory practice” for determination of reliable equilibrium data. During the first period, probably a specific workshop/conference could be organized within existing conferences (e.g. ISMEC). The WG2 meeting(s) will be organized within the NECTAR meetings.

WG meeting(s): 2

Workshop/conferences: 1

STSM(s): 2 - 5 (depending on budget and start of a real collaborative work)

Training schools: 1 (if considering the whole Action)

ITC conference grant(s): 1 - 2

WG3: NECTAR for multicomponent solutions and complex matrices.

Reported by: Slobodan Gadžurić (RS)

MC members preliminarily listed as members of the WG (in alphabetical order):

Sabriye Aydinoğlu (TU), Urte Bubniene (LT), Elvira Bura-Nakić (HR), Angela Casini (DE), Isabel Cavaco (PT), Eva Freisinger (CH), Sofia Gama (FR), Enrique García-España (ES), Iwona Lakomska (PL), Přemysl Lubal (CZ), Vilko Mandić (HR), Alberto Martinez (BE), Demetrio Milea (IT), Igor Povar (MK), Arūnas Ramanavičius (LT), Stefan Stürup (DK), Matteo Tegoni (IT), Oreste Todini (BE), Tatjana Trtić-Petrović (RS).

Summary of the Discussion Outcomes:

Session 1: MoU Tasks and Deliverables

During the discussion several tasks, activities and deliverables were defined, in agreement with accepted MoU:

1) Study of new supramolecular metal-based systems for sensing and biomedical applications;
2) Investigation of interactions in multicomponent systems composed of multiple chelators/ions eg. colloidal systems, biological fluids;
3) Methods improvement and determination of equilibrium constants and thermodynamic parameters in new multicomponent homogeneous and heterogeneous systems;
4) Critical evaluation and prediction of thermodynamic parameters using advanced computational methods and experimental validation;
5) Thermodynamics and kinetics of nanoscale systems;
6) Study of non-aqueous systems and their possible application in medicine and environmental protection.

Session 2: Using the COST Networking tools in the next 12 - 18 months

- 1-2 WG meetings
- 1 Workshop/Conference

- 2-4 STSMs

Several goals were defined for the corresponding period:

1) Writing of annual report
2) Promotion of the research activities especially in ITCs, non-involved countries and among young researchers
3) Inclusion of other COST countries
4) Update of the progress in WG3 on the COST web site
5) One critical review paper on the state-of-the-art in this field and computational and experimental thermodynamic data
6) Special issue of one peer reviewed journal dedicated to the activities and research in WG
7) Exchange of the existing knowledge – upload papers on COST web page and any disseminate results and progress of any kind in our research area

WG4: NECTAR tools, services and facilities.

Reported by: Aleksandar Cvetkovski (MK)

MC members preliminarily listed as members of the WG (in alphabetical order):

Alberto Becares (BE), Axel Buchholz (DE), Angela Casini (DE), Aleksandar Cvetkovski (MK), Montserrat Filella (CH), Sofia Gama (FR), Přemysl Lubal (CZ), Demetrio Milea (IT), Igor Povar (MK), Oreste Todini (BE), Matteo Tegoni (IT), Arūnas Ramanavičius (LT).

Summary of the Discussion Outcomes:

In agreement with MoU, the following objectives were defined for 4 years term:

1) Setting up a platform for a future NECTAR's database based on the collected experimental and calculated thermodynamic parameters;
2) Setting up collaborations with research groups from Academia and Industry with focus on development of analytical methods for measuring thermodynamic parameters;
3) Setting up collaborations with research groups from Academia and Industry for the development of smart compounds and materials for specific purposes;
4) Setting up network collaborations with IT (information technology) sector.

Milestones:

To Objective 1: to collect and get access to thermodynamic parameters based on experimental datasets/results; to calculate thermodynamic parameters for non experimentally accessible results; to apply chemometric methodology/tools to compare, validate and optimize the theoretical and calculated data with experimental results/datasets, in collaboration with research groups that deal with computational chemistry.

To Objective 2: to provide tools for the use of "unconventional" techniques to derive thermodynamic data and/or to interface/couple different instruments/techniques; to optimize and setup recommended protocols/guidelines for: i) correct use of different single and coupled instrumental techniques; ii) experimental data treatment (least-square regressions, linearization procedures, PCA and other chemometric tools); iii) evaluation of calculated data and of speciation models.

To Objective 3: to design, synthesise and characterise new molecules and functional materials (sensors for different applications, compounds of life-science relevance, ingredients for consumer products, etc.) on the basis of available thermodynamic data.

To Objective 4: to develop software and computer tools for: i) data collection (possibly customisable software to be adapted to different laboratories); ii) data analysis and visualization of results. Development/optimisation of *in silico* modelling for the study of the stability of metal/ligand and substrate/receptor adducts; validation of the results using experimental data. Design and management of a database (web-based) for the deposition and retrieval of thermodynamic data (especially equilibrium constants).

To Objective 4: to provide calculation tools for data analysis (e.g. coming from different techniques), for experiments management (e.g. simultaneous data acquisition and instruments managing in coupled techniques).

Session 2: Using the COST Networking tools in the next 12 - 18 months

Objectives:

1) Identifying and prioritising the most critical laboratory practices and data analysis procedures for the determination of thermodynamic parameters that need most urgent revision.
2) Identifying the characteristics of both the platform and the database (of thermodynamic parameters) itself.
3) Selecting analytical instruments/techniques for improved and real-time measurements of process parameters that are used for the determination of thermodynamic parameters.
4) Identifying the chemical-physical and structural characteristics that some molecules should have to be successfully employed in some selected fields.

Milestones:

a) To map and review available software for both data acquisition and analysis;
b) To analyse the pros and cons of the existing databases of thermodynamic parameters;
c) To identify and enrole WG4 members with background in software engineering;
d) To build-up networking with companies and academic research groups for software development;
e) To collaborate with manufacturers of analytical instruments for measurements;
f) To provide optimised syntetic procedures for the production of specific molecules and/or classes of molecules.

Networking tools needed:

Annual/WG Meeting in order to get inputs by reliable WG (especially WG1-3)

Conferences/ Fairs in ITC & chemical sectors/ software development for databases and for analytical techniques for measurements chemical parameters.

WG5: NECTAR for the future: new trends and exploitation of results.

Reported by: Isabel Cavaco (PT)

MC members preliminarily listed as members of the WG (in alphabetical order):

Urte Bubniene (LT), Axel Buchholz (DE), Natalia Busto (ES), Isabel Cavaco (PT), Eva Anna Enyedy (HU), Eva Freisinger (CH) Montserrat Filella (CH), Slodoban Gadžurić (RS), Sofia Gama (FR),

Elżbieta Gumienna-Kontecka (PL), Olga Iranzo (FR), Demetrio Milea (IT), Igor Povar (MK), Arūnas Ramanavičius (LT), Matteo Tegoni (IT), Katalin Varnacy (HU), Emel Yildiz (TU).
Summary of the Discussion Outcomes: Session 1: MoU Tasks and Deliverables The tasks and activities planned for WG5 in MoU were revised, accepted and grouped into 5 separate objectives: 1) Organization of meetings, to favor contacts between research groups. 2) Creation of a website and a presence in social media. 3) Collecting and publishing/disseminating the "Good Practices on the Determination, Analysis and Use of Thermodynamic Data" using the information and results provided by WG1-WG4. 4) Outreach to society and industry: promoting awareness of the importance of good thermodynamic data. 5) Promote and increase academia-industry link, namely through the commercialisation of the products of research. Session 2: Using the COST Networking tools in the next 12 - 18 months *Goals for the next 12 - 18 months:* a) Setting up the project website, by December 2019. Also create dedicated accounts in Facebook, Twitter, LinkedIn and Instagram, and probably a discussion topic in Reddit and/or Quora. Creating a mailing list for internal communication. b) Organizing 2/3 meetings. c) Identify main concerns to be covered in "Good Practices on the Determination, Analysis and Use of Thermodynamic Data". Collect insights from participants on what are the important topics to be covered and define structure and type of publication(s). d) Prepare flyers to be distributed in conferences - by February 2020. e) Define the project Logo - by November 2019. f) Preparing an International Conference. g) Organize an effective system for distribution of information among the action participants. *Networking tools needed:* WG meetings: 1-2 presencial meetings at the time of the MC meetings. Dissemination: participation to 2 selected international conferences/fairs as Action ambassadors.

b. Management of the COST Action

After an introduction on the tasks of the Management Committee for managing COST Actions, the participants divided into groups to discuss and make proposals for different management aspects:

1. Manage requests to join the Action
2. Decide who to invite and reimburse for Action meetings
3. Implementing STSMs
4. Communication Strategy
5. Plan your first Grant Period
6. Implementing ITC Conference Grants
7. International Cooperation
8. Organising Training Schools
9. Stakeholder engagement

The results can be found in Annex 6.

The Management Committee will develop further the ideas into internal rules and procedures of the COST Action.

c. Other points of Discussion

No other point was found to be revevant to be further discussed.

6) Decisions by the Management Committee

From the 20 COST countries parties of the Action (on the 2nd October), 17 were represent by its corresponding MC members. Malta, Iceland and Slovenia were not present. All decisions were approved unanimously (17 votes).

a. Election of the Chair and Vice-chair

Decision 1: Demetrio Milea (IT) was elected Chair
Decision 2: Sofia Gama (FR) was elected Vice Chair

b. Selection of the Grant Holder (Scientific Representative) and agreement of FSAC

Decision 3: The MC selected **Università degli Studi di Messina (IT)** as Grant Holder Institution, represented at the MC by the elected Chair. Upon request of the elected Chair, the MC agreed to award the maximum FSAC rate of 15% of the total Scientific Expenditure.

c. Establishment of Action Management Structure

Decision 4: The following MC members were elected to the leadership positions:

- WG1 leader / co-leader: **Montserrat Filella (CH) / Olga Iranzo (FR)**
- WG2 leader / co-leader: **Petr Hermann (CZ) / Maria Amélia Santos (PT)**
- WG3 leader / co-leader: **Slobodan Gadžurić (RS) / Arūnas Ramanavičius (LT)**
- WG4 leader / co-leader: **Aleksandar Cvetkovski (MK) / Winfried Plass (DE)**
- WG5 leader / co-leader: **Isabel Cavaco (PT) / Natalia Busto (ES)**
- STSM Coordinator: **Matteo Tegoni (IT)**
- Science Communication manager: **Elżbieta Gumienna-Kontecka (PL)**
- ITC Conference Grant Coordinator: **Emel Yildiz (TR)**
- Training School Coordinator: **Enrique García-España (ES)**
- Industry Transfer Manager: **Oreste Todini (BE)**
- Equal Opportunities Manager: **Eva Anna Enyedy (HU)**

Decision 5: The MC decided that the Action Chair (AC), Action Vice Chair (AVC), Science Communication Manager (SCM), STSMs Coordination Manager (STSMCM), TSs Coordination Manager (TSCM), Industry Transfer Manager (ITM), ITC Coordination Manager (ITCCM), Equal Opportunities Manager (EOM), WG(1-5) Leaders will form the Core Group for the daily management of the Action.

Decision 6: The MC decided to mandate the Core Group for any budget change below 10.000 euro, to limit the time for accepting invitations to 10 days, and to monitor the activities of the WGs. Any other specific mandate from the MC to the Core Group will be discussed and decided in the upcoming months.

Decision 7: The MC approved the following decision with regards to the constitution of Committees:

- Coordinators/Managers may decide to appoint some people to support them in performing various activities, creating small Committees.
- If formed, Committees members' names must be communicated / reported to CG (and then to MC)
- Coordinators/Managers have the possibility to appoint / replace committee members at any time during action, just reporting their choice to CG.
- Independently of the presence of a Committee, the ONLY responsible is the Coordinator/Manager, who is the ONLY person officially entitled to report to CG (and MC)
- Analogously, WG Leaders, supported by Co-leaders, may create Committees within WGs, with the same rules as above mentioned.

7) Further decisions

Decision 8: The MC agreed on the following distribution for the WBP for the Grant Period 1, starting the 1st Nov 2019:

Budget: 50'000 EUR (20 countries)

- 1 joint MC, CG and WGs meeting (Feb/Mach 2020, preferably in one ITC)
- STSMs (3)
- Dissemination Activities (Website, social media, other…)

8) Next meeting and Closing

The MC agreed to decide in the next 2 weeks the location of the next meeting. 2 locations in ITC countries were offered by MC members from PT and RS, in the period Feb-March 2020 (to be decided) for a joint MC+CG+WG meeting.

The hosting team gave some final words about the COST Action. The participants expressed their individual follow up actions for the success of the Action.

The MC Chair thanked the participation of all the MC members and closed the meeting at 17.20h.

9) List of Annexes

- Annex 1 - Agenda
- Annex 2 - Presentation from COST Association and Main Proposer/Elected Chair (attached)
- Annex 3 - A Quick Guide to the COST Networking Tools (attached)
- Annex 4 - A Quick Guide to the Tasks and Decision of the Management Committee (attached)
- Annex 5 - List of participants (attached)
- Annex 6 - Afternoon Discussions

Minutes prepared by:

- *Action Science Officer*
- *Action Chair*
- *Action Vice-Chair*

ANNEX 1- AGENDA

- Welcome by the hosting team
- COST Excellence and Inclusiveness Policy
- Tour de table: What am I looking for in this COST Action?
- Presentation of the COST Action by the Main Proposer: Challenge and MoU Objectives, Deliverables, General Action Structure (WGs, Horizontal Tasks, management…), SC recommendations
- Discussion on the MoU (Open Space): Working Groups tasks and deliverables
- Presentation on How COST Actions Work
- Discussion on the use of COST networking tools for financing the Action activities
- Reimbursement Rules
- How to Manage COST Actions?
- Acceptance by the MC of Rules of Procedures for MC of COST Actions
- Election of Chair and Vice Chair; Selection of Grant Holder
- Action Structure and organises the election for the WG and task leaders
- Proposal for WBP for the next Period and Next meeting: date and place
- Final Messages from COST and checkout: What will you start tomorrow to contribute to the success of this Network?