EUROPEAN COOPERATION IN SCIENCE & TECHNOLOGY

Brussels, 4 June 2019

COST 019/19

DECISION

Subject: **Memorandum of Understanding for the implementation of the COST Action "Network for Equilibria and Chemical Thermodynamics Advanced Research" (NECTAR) CA18202**

The COST Member Countries and/or the COST Cooperating State will find attached the Memorandum of Understanding for the COST Action Network for Equilibria and Chemical Thermodynamics Advanced Research approved by the Committee of Senior Officials through written procedure on 4 June 2019.

MEMORANDUM OF UNDERSTANDING

For the implementation of a COST Action designated as

COST Action CA18202
NETWORK FOR EQUILIBRIA AND CHEMICAL THERMODYNAMICS ADVANCED RESEARCH (NECTAR)

The COST Member Countries and/or the COST Cooperating State, accepting the present Memorandum of Understanding (MoU) wish to undertake joint activities of mutual interest and declare their common intention to participate in the COST Action (the Action), referred to above and described in the Technical Annex of this MoU.

The Action will be carried out in accordance with the set of COST Implementation Rules approved by the Committee of Senior Officials (CSO), or any new document amending or replacing them:

a. "Rules for Participation in and Implementation of COST Activities" (COST 132/14 REV2);
b. "COST Action Proposal Submission, Evaluation, Selection and Approval" (COST 133/14 REV);
c. "COST Action Management, Monitoring and Final Assessment" (COST 134/14 REV2);
d. "COST International Cooperation and Specific Organisations Participation" (COST 135/14 REV).

The main aim and objective of the Action is to provide a scientific and technological platform to gather together, under a unique network, a critical mass of European research groups with a strong expertise in chemical equilibria with industrial stakeholders, with the valuable reinforcement of international partners and European enterprises.. This will be achieved through the specific objectives detailed in the Technical Annex.

The economic dimension of the activities carried out under the Action has been estimated, on the basis of information available during the planning of the Action, at EUR 60 million in 2018.

The MoU will enter into force once at least seven (7) COST Member Countries and/or COST Cooperating State have accepted it, and the corresponding Management Committee Members have been appointed, as described in the CSO Decision COST 134/14 REV2.

The COST Action will start from the date of the first Management Committee meeting and shall be implemented for a period of four (4) years, unless an extension is approved by the CSO following the procedure described in the CSO Decision COST 134/14 REV2.

OVERVIEW

Summary

The thermodynamic study of chemical equilibria represents the core of many important branches of chemistry. Coordination and supramolecular chemistry, chemical speciation, molecular modelling, drug design are just few examples. The importance of chemical equilibria, and chemical thermodynamics in general, results from the simple assertion that many properties of elements and compounds depend mainly on their interactions in a given system: the biological activity of an element or molecule, or their environmental impact can be explained by a detailed study of these interactions, whose nature and strength can be evaluated by chemical equilibrium and other thermodynamic studies. For example, speciation modelling based on chemical equilibrium data is commonly used in to improve commercial products performances, investigate the mobility of pollutants and toxicants in the environment, optimize industrial processes, explain the mechanisms of action of biologically active substances. Furthermore, advanced thermodynamic studies yield deeper insights into the mechanisms of these interactions.

NECTAR will combine the expertise of the large community of specialists working in this field, creating a network based on the stimulating collaboration between them, promoting knowledge exchange, and achieving high technological progress. All this will be accomplished through a fruitful collaboration between young researchers and experienced scientists, taking into consideration gender balance and maximal geographical distribution. Innovative and integrated theoretical and experimental approaches will be established and optimized. Overall, the outstanding quality of obtained results will serve as benchmark for next decades, allowing their application in the above-mentioned fields and substantially impacting on life quality of next generations.

Areas of Expertise Relevant for the Action	**Keywords**
● Chemical sciences: Analytical chemistry	● Chemical Thermodynamics
● Chemical sciences: Coordination chemistry	● Chemical Equilibria
● Chemical sciences: Supramolecular chemistry	● Coordination Chemistry
● Chemical sciences: Method development in chemistry	● Complexes
● Chemical sciences: Chemical instrumentation	● Stability Constants Databases

Specific Objectives

To achieve the main objective described in this MoU, the following specific objectives shall be accomplished:

Research Coordination

● Give response to actual scientific and technological challenges. In the wide field of equilibrium thermodynamics, particular attention will be paid to four specific areas: i) biology and medicine; ii) environmental science; iii) technology and industry; iv) modelling and software development.

● Develop new technologies. The multidisciplinarity and diversity of expertise within NECTAR will bring about a demand for developing new technological solutions, which will successfully combine all stakeholders' interests.

● Identify new industrial stakeholders and applications. One of NECTAR's aims is to enlarge the perception about the potential of the use of different thermodynamic studies on specific industrial and technological applications (including environmental and biological/medical).

Capacity Building

● Promoting mobility and multidisciplinary training between the different participants of the Action.

● Transfering knowledge and promoting industrial awareness.

● Supporting a high proportion of ECIs, ITCs and assuring gender balance in the COST Action

● Promoting the sustainability of the network beyond the Action.

TECHNICAL ANNEX

1 S&T EXCELLENCE

1.1 SOUNDNESS OF THE CHALLENGE

1.1.1 DESCRIPTION OF THE STATE-OF-THE-ART

The research on chemical equilibria embraces all areas of chemical sciences. The fundamental knowledge of the thermodynamics of chemical processes has a tremendous impact on many disciplines such as biology, medicine, environmental sciences, agriculture and engineering. The study of chemical equilibria plays a pivotal role through the design and synthesis of chemical compounds, their characterization and determination of their physico-chemical properties, as well as their exploitation for specific applications. On one hand, the wide interdisciplinarity of thermodynamic studies of chemical transformations and the myriad of different applications all combine to place the research in this field always at the cutting edge. On the other hand, these two aspects both concur to create a bottleneck for the coherent and harmonic development of a comprehensive theoretical and experimental approach to the thermodynamic study of any chemical system. In the last century, many studies were performed on solution thermodynamics and much useful technology has been developed in this area. Up to the 1960s, the main aim was the determination of equilibrium constants, as well as the development of reliable methodologies for this purpose, including instrumentation and methods for data analysis. All this contributed, shortly afterwards, to the development of the new research field of **Chemical Speciation**, which exploits chemical equilibrium data to define the distribution of a given component in a given system among its different species. These studies gave a real boost to research in the field of solution chemistry. Substantial advancements were made in the 1970s and 1980s through the optimisation of new instrumental techniques and the development of computer-aided calculation tools. Moreover, the implementation of a series of stability constants (and other thermodynamic parameters) databases under the coordination of internationally recognised organisations (e.g., IUPAC, NIST) has underpinned research in a vast number of fields. In the last two decades there has been an explosion of published thermodynamic data for specific systems in specific conditions. The availability of new tools to perform these studies (e.g., automated instrumentation, dedicated software) provided easy access to these thermodynamic data also for investigators without a solid background in the field. Consequently, much of the published data did not undergo a critical and rigorous analysis and hence provided not always undisputable interpretations of chemical phenomena. Studies on solution equilibria started then to take a back seat, since the number of low quality/routine results increased and published data not always fulfilled the required quality standards. As a consequence, solution chemistry was relegated to an area which is intended to provide only additional data instead of the key information necessary to challenge a chemical problem, pushing at the same time *pure* solution chemists to look for different and *trendier* research fields. Concerning that, as early as 1992, Martell and Motekaitis, in their fundamental book "Determination and Use of Stability Constants", warned the scientific community stating that "the proliferation of publications in this field, by which investigators would report stability constants for their own sake, without any apparent objective of advancing the concepts and principles of coordination chemistry, or of providing information essential to other fields, has led to a general decline in the prestige of this research area, and work on stability constants gradually came to be regarded as routine". Unfortunately, to the detriment of Science, after nearly thirty years the situation remains unchanged. Few improvements have been observed in providing non-specialists and beginners with training and/or easy and reliable methods for the study of chemical thermodynamics and, concurrently, solution equilibria are less frequently considered in University teaching programs. Also, some organisations

(IUPAC, NIST) that for decades have maintained and updated the stability constants databases have recently dismissed this service. Consequently, not only the retrieval of thermodynamic parameters has become more difficult, but also no downstream critical data analysis was possible after publication. Nevertheless, several research groups in academia and industry are still focused on the rigorous investigation of the thermodynamics of chemical equilibria. This study is conducted on systems of interest in the most diverse areas of basic and applied research, and additionally in the development of new methodologies, software and apparatus. Certainly, the wide spread use of the techniques for the analysis of equilibria in solution had positively impacted many research areas, such as host-guest interactions, supramolecular aggregates, biological macromolecules, polymeric systems and molecular machines. However, the huge amount of thermodynamic data produced nowadays are often useful only for the characterization of specific systems and useless or not interesting for a wider audience. Quite paradoxically, these circumstances are sometimes the simple result of wrong experimental setup or errors in the procedures for data treatment resulting from a limited expertise in the field. New fundamentals of both the theoretical and experimental approaches to the thermodynamic study of these systems need to be developed. Also, new advances are required to fulfil the need of a deeper comprehension of the physico-chemical properties of systems that, year after year, increase in complexity. Finally, and perhaps most importantly, several aspects in solution thermodynamics scarcely considered in the past demand nowadays a deeper attention. Among these: i) the study of secondary interactions (e.g., weak complexes or ion pairs, competing reactions in real systems); ii) the systematic analysis of particular systems to derive general information (e.g., the systematic study of the complexing ability for ligand classes); iii) the kinetic aspects of some particularly slow complex formation processes; iv) a rigorous analysis of the literature data; v) the construction and/or the implementation of suitable general databases; and vi) the parallel investigation of other parameters than those strictly of interest.

1.1.2 DESCRIPTION OF THE CHALLENGE (MAIN AIM)

The overriding goal of NECTAR is to provide a scientific and technological platform to gather together, under a unique network, a critical mass of European research groups with a strong expertise in chemical equilibria with industrial stakeholders, with the valuable reinforcement of international partners and European enterprises. As such, NECTAR ambitiously aims to connect the widest possible number of subjects whose competences and resources may provide significant advancements in the field of the thermodynamics of chemical equilibria. By exploiting the complementary skills and research fields of various partners, as well as the different nature of involved institutions (e.g., universities, research centres, and enterprises), this network will allow the participants to address specific issues and needs in the field of chemical equilibria. Besides these research coordination goals, capacity-related objectives will be pursued. The latter will be primarily the transfer of knowledge between fundamental research to applications and, importantly, the training of early-stage researchers. As for the transfer of knowledge, we believe that COST is the perfect framework for the involvement of stakeholders, since the latter will participate to discussions offering their perspectives and highlighting their needs. On the other hand, the training of early-stage researchers is more effective when carried out within the framework of a European network that offers a large number of competences and facilities accessible through short-term scientific missions (STSMs) and training schools (TSs). Through this networking activity, NECTAR will surely represent the most concrete and ideal environment where key topics related to equilibrium analysis and chemical thermodynamics will be examined. Particular focus will be on:

i) The study of chemical equilibria of complexes with highly hydrolysable (HHC) and/or low valence state (LVC) cations. This Action aims at providing reliable, accurate and comprehensive sets of thermodynamic data for systems of interest in biological, environmental and technological/industrial areas. Protocols and new methodologies for the study of these cations will be provided.

ii) The optimisation of instrumental methods and data treatment procedures for the study of chemical equilibria in systems where very strong or multivalent/multisite interactions between components occur. These activities will be of particular interest, for instance, in biomedical applications (e.g., chelation therapy, nuclear medicine, metal complexes with macromolecules) or environmental sciences (e.g., remediation, *precious* metal recovery, waste processing and water treatment).

iii) The setup of experimental and data treatment protocols for speciation studies of multicomponent systems or in non-conventional solvents or mixtures. These activities will address the issues connected with the speciation of systems where, for instance, multiple metals and ligands are present in solution. Also, systems in ionic liquids, mixed solvents, systems containing surfactants or sorbent materials will

be considered. These systems are of interest for the study of natural waters, biological fluids, industrially/technologically relevant systems, commercial/consumer products, etc..

iv) The optimisation of the protocols for the use of coupled experimental techniques, and related data treatment (e.g., potentiometry/spectrophotometry).

v) The development of new suitable and customisable software for data acquisition with different techniques, and for experimental data analysis and calculation tools.

vi) The study of the stability of complexes using *in silico* approaches. The determination of the molecular structure of complexes using theoretical calculations and their correlation with experimental data. The modelling of the dependence of thermodynamic quantities and/or speciation on systems' conditions (e.g., composition, ionic strength, temperature).

vii) The review and upgrade of existing thermodynamic databases and, eventually, the setup of new ones.

NECTAR will take advantage of the networking activity at a European and ultimately global level, and will represent the ideal framework to share information and technologies between partners, and to establish new projects and collaborations to solve the current main challenges in the study of chemical thermodynamics. Through the involvement of stakeholders and training activities NECTAR will ultimately provide the best framework for maximising capacity-oriented outcomes, bridging the historical gaps between basic and applied research with mutual and durable benefits for science and society.

1.2 PROGRESS BEYOND THE STATE-OF-THE-ART

1.2.1 APPROACH TO THE CHALLENGE AND PROGRESS BEYOND THE STATE-OF-THE-ART

The recent scenario in chemical thermodynamics has been to tackle an identified problem focusing almost exclusively on the practical aspects of the problem itself, often resulting in limited impact and success. This approach represents a bottleneck in the advancement of knowledge that is essentially cultural in its nature. NECTAR aims at developing and implementing the vision of matching a strong scientific environment with the objective of strengthening the cultural impact of its activities. NECTAR will provide experimental and theoretical advancements in the field of chemical equilibrium thermodynamics. These will be in the form, for instance, of formulation of solid protocols and guidelines for the experimental study of chemical equilibria, the development of calculation techniques for data treatment, the realization of dedicated software and computer tools, the creation and maintenance of databases, the proposition of new theoretical approaches, the design and synthesis of targeted compounds with desired properties and functions on the basis of their stability in solution. Furthermore, and possibly more important from a social and cultural point of view, through the accomplishment of these activities NECTAR wants to reach a level of excellence in *training*, *employing* and, ultimately, *offering* and *delivering* human resources with an outstanding level of competences and knowledge in the field of solution thermodynamics and its applications, i.e., it aims to produce new *thermodynamic minds*. This is the only possible strategy to ensure that this research will be performed again by trained scientists, and that its results and findings will correctly be *handled* by experts in the field. This will bestow again on this discipline the socio-economic impact and its crucial role in ameliorating the quality of life by providing concrete and valuable services deriving by the technological and scientific innovations obtained through advancements in solution thermodynamics. Hence, to bring research on the thermodynamics of chemical equilibria back again to the level it deserves among the scientific community and the public opinion, through this young and innovative approach NECTAR aims to promote effective and durable actions, both at a technical and cultural level.

Share, Communicate and Disseminate. The interdisciplinary nature of chemical thermodynamics, the wide number of applications, the diverse issues to solve, the different points of view to tackle various challenges, and the diverse background of researchers, have all contributed to the above-cited fragmentation and heterogeneity of approaches and results. In the era of communication and global information, it is incongruous and illogical how information and main findings in this field are compartmentalized and restrained into closed-door environments. Similar systems unintentionally investigated by different groups, difficulties encountered in one sector that have been solved in another, facilities necessary in one place that are easily available in another, are just few examples. The

limitations caused by this lack of information and awareness can be easily solved by more efficient knowledge sharing and communication between the leading research groups investigating or exploiting chemical thermodynamics at various levels, but also institutions, enterprises, governments and all subjects interested in ameliorating the society.

Identify and Develop. Whoever deals with thermodynamics of chemical equilibria should identify what are the interests and the skills that link or differentiate each other in their specific sectors, with the aim of developing shared strategies to tackle various issues in an integrated approach. Harmonization of common know-how and exploitation of complementary competences and skills are highly desirable. New guidelines should be proposed, discussed and approved for the use of standardized and recommended experimental procedures and theoretical approaches, in order to reach high quality / excellence standards in the entire field of chemical thermodynamics. The widest consensus possible in the community of researchers is advisable, for instance, on the strategies for the assessment of the concentration and purity of the analytes, on the procedures for the determination of high-quality data, on the nature and quality of databases, on the level of accuracy of models obtained by *in silico* studies to support the interpretation of experimental data in chemical equilibria.

Train and Deliver. The well-known (and always valid) computer science motto of "Garbage-In Garbage-Out" perfectly holds also for chemical thermodynamics. Actually, researchers working *in* this field need high-quality data to obtain high-quality results. Analogously, also subjects working *with* (i.e., using) chemical thermodynamics need high-quality data and models to obtain high-quality performances of what is produced by those data (in terms of both material goods and services). The only possible way to reach this level of excellence as fast as possible is to train people dealing with this discipline to an outstanding standard level, by promoting good laboratory practice and excellent theoretical background. Only very well-trained people will be able to deliver their great experience and outstanding skills to whatever subject will request them: academy, research centres, enterprises, governments and other institutions.

1.2.2 OBJECTIVES

1.2.2.1 Research Coordination Objectives

NECTAR will promote coordinated and collaborative research activities by stimulating and encouraging networking, ultimately assuring the growth of the scientific strength of all parties involved, which is crucial for the success of the related tasks. Progressive and innovative research competences are needed, and this will be only possible by a diverse but concerted effort and a concentrated expertise of a critical mass of outstanding researchers. In this light, NECTAR will bring together a large number of participants from different countries and research areas, from experimentalists to theoreticians and instrumentalists, all interested in the field of chemical thermodynamics. The melding of different skills will be promoted by creating a vast knowledge background able to respond to all the scientific and technological demands of both the scientific community and the stakeholders. Collaborative research among members of the Action Network will be endorsed, favouring the mutual understanding and the dialogue between scientists from different fields, and largely improving the profit of joint efforts. Synergies with other Actions will be also encouraged, together with the participation in EU programs, thus giving NECTAR an active role in networking at an international level. The success and stimulation for research is highly connected with the communication and dissemination of results and the sharing of knowledge with other communities. This is essential to step up the research progress, and will be the basis of all the networking activities of NECTAR: the promotion of scientific achievements not only boosts the visibility of the existing scientific and technological challenges, but also promotes the awareness of their importance for industrial interests and European policies. This will be achieved by the following partial task objectives during the Action:

Give response to actual scientific and technological challenges. In the wide field of equilibrium thermodynamics, particular attention will be paid to four specific areas: i) biology and medicine; ii) environmental science; iii) technology and industry; iv) modelling and software development. Understanding experimental evidences is a challenge that NECTAR intends to address by developing new experimental strategies and methods, based on chemical equilibrium and other thermodynamic studies. These goals require bringing together basic and applied science. The accomplishment of this objective will necessarily pass through the success of Working Groups (WGs) 1-3 in solving their specific tasks through their activities.

Develop new technologies. The multidisciplinarity and diversity of expertise within NECTAR will bring about a demand for developing new technological solutions, which will successfully combine all stakeholders' interests. NECTAR aims, with the support of manufacturers, to improve existing, and develop new, experimental techniques for the study of chemical equilibria, ultimately making available analytical tools able to cope favourably with the identified scientific problems to be solved. Besides the clear advantage in terms of scientific progress and development inside the Action, this will also be a way to promote commercial applications, thereby resulting in intellectual property rights, all of which fall under NECTAR´s fundamental goals. In this respect, the involvement of stakeholders can promote the attention of research groups toward the patentability of the obtained foreground, with a positive impact on economic aspects (see also below). Activities carried out by WG4 to solve its tasks will fulfil this objective.

Identify new industrial stakeholders and applications. One of NECTAR's aims is to enlarge the perception about the potential of the use of different thermodynamic studies on specific industrial and technological applications (including environmental and biological/medical). This will be promoted by the activities of a dedicated Working Group (WG5) and through an active focus on improving the communication between scientific community, institutions, industry and society. On one hand, the recognition of key industrial applications and subjects of which the scientific community is still not aware of will be an objective. On the other hand, NECTAR will operate to bring the necessary background on chemical thermodynamics to institutions and industries, making them aware of all the scientific possibilities for solving specific problems. For this, the scientific communication and dissemination already described are crucial.

1.2.2.2 Capacity-building Objectives

The NECTAR Action is focused on one main capacity-building objective: to create a solid, recognized and sustainable network where different challenges and interests are approached from a wide perspective, after the recognition of mutual benefits between research centres, industries, institutions and general public. This main goal can be achieved carrying out different actions, such as:

Promoting mobility and multidisciplinary training between the different participants of the Action. The interaction between all NECTAR participants will be promoted in several ways, namely by the Action official website, the organisation of annual meetings where several presentations will take place, together with fruitful discussions within the network community, brokerage events and speed date meetings. To maximize the benefits for all participants, mobility and multidisciplinary training between the different protagonists of the Action will be promoted. This will enable NECTAR members to access different laboratories with different expertise (from completely different techniques to slightly different approaches using the same technical apparatus). This objective will target more specifically Early Career Investigators (ECIs) and Inclusiveness Target Countries (ITCs), with the aim of maximizing trans-national and trans-sectorial mobility. Different activities will take place to achieve this, such as the promotion of STSMs to support ECIs and ITCs researchers to interact with and learn from more experienced researchers, as well as the creation of a structured environment inside the different WGs, which will offer mentoring and guidance to the new researchers, encouraging them to participate in the Management Committee (MC), WG meetings and plenary sessions. This will result in the gain of experience in several fields and will promote project leadership especially among young scientists.

Transfering knowledge and promoting industrial awareness. Many NECTAR activities will be focused both on increasing the consciousness for the potential use of chemical thermodynamics in different technological fields, and on attracting not only new scientists, but industrial investors and technological developers too. Partnerships with manufacturers and other stakeholders will be particularly important also to test, in different scientific environments, the apparatus and approaches developed through NECTAR Action. Scientific publications, outreach activities (especially talks by expert Action members and open-day events), the Action website and the organisation of international meetings will be some of the strategies that will be used for the communication and dissemination of guidelines and scientific results. This will develop strong links between industry and academia at an international level and promote a trans-boundary transfer of knowledge.

Supporting a high proportion of ECIs, ITCs and assuring gender balance in the COST Action. NECTAR members will focus on encouraging ECIs, ITCs and female researchers to actively take part in leading and managing the Action focusing, in particular, on the organisation and participation in TSs, STSMs

and WG meetings. Likewise, they will be also addressed with some of the leadership positions, one important step concerning efficient career development plans.

Promoting the sustainability of the network beyond the Action. NECTAR will establish solid and sustainable synergies through the implementation of research projects in the chemical thermodynamics area at the trans-national level. This will spread interest and knowledge not only within the academic community but also at an industrial and institutional level, including scientific associations. We preview that this will be achieved, for instance, by encouraging network members to develop collaborative funding applications (e.g., EU programs) and by maintaining the planned Action website as a sustained open resource for researchers and industry.

2 NETWORKING EXCELLENCE

2.1 ADDED VALUE OF NETWORKING IN S&T EXCELLENCE

2.1.1 ADDED VALUE IN RELATION TO EXISTING EFFORTS AT EUROPEAN AND/OR INTERNATIONAL LEVEL

To the best of our knowledge, there currently is no European or other international network similar to NECTAR, dedicated to chemical equilibrium thermodynamics at a so vast, multidisciplinary and multipurpose in scale. The field is of such a broad interest that many other programmes and projects have been funded both recently and in the past, though the majority is dedicated to topics addressing the thermodynamic aspects of chemical equilibria only marginally or, in contrast, too specifically. Limiting the list to COST Actions, we can cite: CM1005 (Supramolecular Chemistry in Water, 2011-2015) and D11 (Supramolecular Chemistry, 1999-2003) dedicated to supramolecular chemistry; CM1105 (Functional metal complexes that bind to biomolecules, 2012-2016), D39 (Metallo-Drug Design and Action, 2006-2011), D38 (Metal-Based Systems for Molecular Imaging Applications, 2006-2011), D21 (Metalloenzymes and Chemical Biomimetics, 2000-2006), D20 (Metal Compounds in the Treatment of Cancer and Viral Diseases, MCCV, 2000-2006), D18 (Lanthanide Chemistry for Diagnosis and Therapy, 2000-2006), D8 (The Chemistry of Metals in Medicine, COMM, 1997-2001), addressed to the role of metal complexes in biology and medicine; CM1203 (Polyoxometalate Chemistry for Molecular Nanoscience, PoCheMoN, 2012-2016), D14 (Functional Molecular Materials, 2000-2005), D31 (Organising Non-Covalent Chemical Systems with Selected Functions, 2004-2009), ES1407 (European network for innovative recovery strategies of rare earth and other critical metals from electric and electronic waste, ReCreew, 2015-2019), CM1304 (Emergence and Evolution of Complex Chemical Systems, 2013-2017), TD1407 (Network on Technology-Critical Elements: From Environmental Processes to Human Health Threats, NOTICE, 2015-2019) covering some aspects of materials chemistry, chemical engineering and environmental sciences. These networks dealt or deal with chemical systems through studies of chemical thermodynamics, but none of these specifically focused on the implementation of new methods of studying chemical equilibria. With NECTAR we intend to create, for the first time, a platform where all the different topics and fields of application of chemical thermodynamics can be addressed. Topics that were in the focus of above-mentioned actions would now be explored and investigated from a detailed thermodynamic point of view. For example, an exhaustive comprehension of the chemical thermodynamics of some specific metal complexes (from the determination of their stability constants to their speciation in real systems) is fundamental for the interpretation of their activity in biological systems. This is of enormous relevance when we want to know or explain how metal complexes bind to biomolecules (CM1105), how a particular metallo-drug acts (D39, D20) or how to mimic metalloenzymes (D21). On a strict technological ground, thermodynamic equilibria are also extremely important when considering the design of new “Functional Molecular Materials” (D14) or “Polyoxometalates for Molecular Nanoscience applications” (CM1203), or when dealing with “technologically critical elements” (TD1407). Likewise, chemical speciation is fundamental to issues related to environment and chemical engineering (CM1304). Accordingly, NECTAR will enhance the interest of the scientific community for the potential of this research field in a broad manner, catalysing new and innovative studies. This leads us to say that, for the first time, an Action will merge different areas (from biology and medicine to environment and technology) in a deep and highly integrated mode, based on a common interest: chemical thermodynamics.

2.2 ADDED VALUE OF NETWORKING IN IMPACT

2.2.1 SECURING THE CRITICAL MASS AND EXPERTISE

The strength of NECTAR Action lies in the wide expertise, number and diversity of the proposers, in addition to their geographical and age spread. An extensive and interdisciplinary network involving experts in main areas of chemistry (mainly, but not exclusively, analytical, environmental, inorganic, medicinal, physical and organic), other than chemical engineering and biology will virtually guarantee the availability of skills in all areas required to achieve the goals of the Action. As at submission, the network will have an estimated number of 52 proposers from different Organisations (Higher Education & Associated, Governmental/Intergovernmental and Standard) and 3 enterprises (2 SMEs and 1 large company), based in 15 COST countries (from which 8 are COST ITCs: 53.3%), 1 Near Neighbour Country (NNC) and 2 International Partner Countries (IPCs). Several researchers belonging to these Organisations have, in small clusters, already collaborated in the past on specific scientific subjects. However, none of these clusters had the potential to challenge either the general or specific tasks of this project. On the contrary, by networking these experts and stakeholders it will be possible to exploit all the potential of the EU in this scientific area, and to boost the impact of the contribution of the European research in this field at the top world level. The appropriate funds for research will be guaranteed by the numerous ongoing national and international financed projects, in which the associated scientists of this proposal are involved. This will enable the efficient use of network resources to the benefit of all parties involved. From a global perspective, this consortium will offer virtually all core expertise required. In addition, all partners, including IPCs and NNCs, will profit from networking with state-of-the-art laboratories as well as the strong and successful research collaborations. It is anticipated that the NECTAR Action will, at some stage, undergo expansion not only among other Organisations and countries in Europe , as well as IPCs)and NNCs. At the same time, industrial stakeholders and especially the technology developers already involved in the consortium will be able to take advantage of the networking activity by providing technological tools that can be tested by a wide pool of researchers. This will help to develop technologies that are of interest to a large number of potential users, and are to be continually updated based on the latest *market* needs. Also, this NECTAR group of researchers has the opportunity to be in constant contact with companies available to provide all-round service for them, developing dedicated, customised and customisable solutions for their research. Furthermore, special attention will be paid to the communication with other SMEs and leading companies, in order to strengthen their involvement in the consortium. Lastly, as previously stated, increased contribution of industral partners in the network will be pursued. This is a very achievable point, as revealed in the already existent (and fruitful) interaction of many of the proposers with SMEs (e.g., software development companies, fine chemical suppliers), as well as multinational enterprises.

2.2.2 INVOLVEMENT OF STAKEHOLDERS

This Action identifies three broad groups of stakeholders: core chemistry research groups, researchers in other scientific disciplines (e.g., environmental sciences, pharmaceutical sciences, biology, medicine, engineering), and industry. Stakeholders can be interested in the activities of this Action at two levels, namely as partners in research and development, or as end users of methods or instrumentation. The minimal criteria for joining NECTAR as partners will be: i) to provide access to the instrumentation for the study of chemical equilibria to the scientific community of this Action; ii) to provide expertise and services, in particular in training ECIs; iii) to collaborate with manufacturers and/or software companies to develop and test new instrumentations, procedures and methods for the study of chemical equilibria. Preliminary contacts allowed to predict that more than 60 Organisations (Higher Education & Associated, Government/Intergovernmental and Standards, and manufacturers or software developers) will be interested in joining this Action as partners from over 18 countries (half of which will be ITCs). However, examining the recent scientific literature and patents, we believe that the number of potential partners far exceeds the number of those that have initially expressed their interest. A specific WG (WG5) in this Action will set up and update a plan for maximizing the communication and the dissemination of the information on the activities of NECTAR, as well as its visibility. The channels used to involve new academic stakeholders from the area of chemistry or from other scientific disciplines will be those of the principal scientific communication and dissemination: participation to conferences, symposia organised within other COST Actions, release of scientific papers. Channels to attract stakeholders from the industry will include press releases and web-based communication (from a dedicated website to social media), joint meetings and brokerage events. Finally, this Action will conjoin

research groups that make an extensive use of up-to-date scientific apparatus and customised software. For this reason, many of the potential participants who have expressed interest for NECTAR already have a tight connection with instrument manufacturers and software developers that will be made aware of the activities of NECTAR. The coordination of research carried out through this Action will reinforce these connections: this will boost the industrial stakeholders to be involved in all relevant activities aimed to test new technology including apparatus, procedures and methods.

2.2.3 MUTUAL BENEFITS OF THE INVOLVEMENT OF SECONDARY PROPOSERS FROM NEAR NEIGHBOUR OR INTERNATIONAL PARTNER COUNTRIES OR INTERNATIONAL ORGANISATIONS

At the moment of the submission of this proposal, partners from two IPCs (USA and Australia) and one NNC (Ukraine) have already expressed great interest and support this action as proposers, which is clearly a strong indication of the quality and potential of NECTAR. They are not only linked by common interest in chemical thermodynamics, but they also bring in the project different facilities and complementary skills, representing a real added value for the whole Action. The USA proposer, from the University of California, Berkeley, is universally acknowledged as one of the leading lights in the field of chemical thermodynamics and, with his outstanding package of skills, experience and knowledge, will be a huge asset for expanding NECTAR worldwide. At same time, being part of NECTAR will allow the US partner to enlarge and strengthen his network of collaborations with European leading groups in the field, to be constantly updated on the cutting-edge research performed in EU and, last but not least, to take immediate advantage of innovations and technologies developed through NECTAR activities. The Australian proposer is from the University of Western Australia, Perth, and he has an outstanding experience in the field of physical chemistry and solution equilibria. Most importantly, he is one of the authors/managers of a powerful research tool for thermodynamic modelling of chemical speciation in complex aqueous environments, other than a large database of stability constants and other thermodynamic data. Therefore, the participation in NECTAR of the Australian partner will at least allow him to have direct access to the latest and more accurate thermodynamic data to maintain and update this chemical thermodynamics database, which is, in turn, one of NECTAR goals. In fact, through networking, this action will exploit the partner's activity to ensure the entire scientific community trust in the robustness of a comprehensive, accurately verified and constantly updated database for stability constants and other thermodynamic data. This is notable since two of the most diffuse databases, i.e., Pettit's (IUPAC) and Martell's (NIST), are no longer updated. Finally, Ukraine will also be part of the initial consortium, represented by two proposers. One is from the Taras Shevchenko National University of Kyiv, one of the preeminent Ukrainian academic institutions with a solid tradition in coordination chemistry, while the other is a company that is now recognised as one of the world leading providers of screening compounds and building blocks, also offering integrated services of custom synthesis, lead optimisation and molecular modelling. The academic partner already has long-lasting collaborations with some other NECTAR proposers' research groups. However, with the inclusion in the consortium, further fruitful collaborations are predicted, namely taking into consideration the high expertise of the proposer on the thermodynamic study of non-conventional systems, one of the main interests on the action. As such, its involvement will surely result in a win-win interaction for both parties. Also, the involvement of such a company among the proposers will allow all NECTAR members to take immediate advantage, since the very first moment, of a series of valuable tools and services that will be necessary to perform some of Action's activities. On the other side, belonging to such a consortium will represent for the company a unique opportunity to exploit an exceptional basin of human resources with outstanding competencies in chemical thermodynamics and coordination chemistry, opportunely balanced among well experienced scientists and talented young researchers.

3 IMPACT

3.1 IMPACT TO SCIENCE, SOCIETY AND COMPETITIVENESS, AND POTENTIAL FOR INNOVATION/BREAK-THROUGHS

3.1.1 SCIENTIFIC, TECHNOLOGICAL, AND/OR SOCIOECONOMIC IMPACTS (INCLUDING POTENTIAL INNOVATIONS AND/OR BREAKTHROUGHS)

The NECTAR action will promote the rise and consolidation of a community of researchers with a high expertise in the study of chemical equilibria, with the aim to develop new methodologies for the study of chemical systems and processes. The activity of this network will be at the interface of core chemistry, biology, environmental sciences, and industrial research, and will provide new technological tools and methods able to impact the research on chemical equilibria and transformations in all these areas. NECTAR aims to involve the principal users and developers of methods for the study of the thermodynamics of chemical transformations (e.g., academia, institutions, industry, manufacturers and software developers). This collaboration will rapidly boost the knowledge in this field beyond the state-of-the-art, by focusing on the nature of the methods to be developed instead on the single system under study. The establishment of standardised procedures between different laboratories, as well as the test of apparatus developed by manufacturers, will rapidly provide the research groups with new and reliable methodologies. In addition, this will help the manufacturers to rapidly develop new equipment and to bring innovative technologies to the market. We foresee the short-term scientific and technological impact as: i) structuring of the widest community, at the European level, of experts in the study of the thermodynamics of chemical transformations and chemical equilibria; ii) training of young (ECIs) researchers through the sharing of expertise and facilities across and outside Europe, through STSMs; iii) identification of problems and challenges both of wide interest for the scientific community studying the equilibria in chemical transformations and/or of more specific interest for stakeholders; iv) coordination of the research of this Action with the aim to tackle these challenges at the top methodological level; v) creation of added value through the distribution of new products (instrumentation, software). The main mid- and long-term scientific and technological impact will be: i) to publish and, in general, to communicate and disseminate in the scientific community new methodologies for the study of chemical equilibria, including the major stakeholders in the area of biology, medicine, environmental sciences and industry; ii) to support further applications for funding and grants to national and trans-national agencies; iii) to develop new apparatus and software for data acquisition and treatment in collaboration with manufacturers and software developers; iv) to train a new generation of experts in this field. As for the social impact, the major benefits will be in the field of the mobility of ECIs within and outside the EU. Their participation in this Action will be of great benefit not only for their career, but also on a cultural ground, since they will have the possibility to spend several weeks in very different cultural environments. Finally, we preview that the greatest socio-economical benefit will be gained by ITCs. Their participation in this project will provide the research groups and stakeholders in these countries with the unique possibility to meet the major experts in the field, opening the possibility to access different markets (for industry) and to apply for funding to major trans-national agencies (for academia). Chemical thermodynamics regulate all chemical transformations, so, for this reason, the knowledge of the equilibrium thermodynamics of chemical reactions is absolutely fundamental in the complete understanding of phenomena that occur in nature and in industrial processes. The members of NECTAR are among the world leaders in this area, and already involved in the study of systems at the interface between chemistry, biology, environmental science, and fine chemicals of interest for chemical industries. Therefore, NECTAR will be a great opportunity to join all this expertise and to focus on key challenges that need to be tackled in a coordinated manner. Specific technical and scientific bottlenecks hamper the possibility to study chemical phenomena that are of great interest for the scientific community (e.g. hard to detect analytes, chemical equilibria to be studied under high or low temperatures and/or pressures, complex matrices, etc.). These bottlenecks were challenged for many years by researchers in this area and still only a few of them have been overcome and solved, at a very slow pace. It is therefore beyond any doubt that only a large scientific community that has a strong connection with instrument developers may speed up the knowledge on these aspects. This will be beneficial for the development of knowledge in the area of interest of all stakeholders. Two principal risks are perceived: 1) the insufficient breadth of expertise needed to tackle the scientific challenges of this project; 2) the Action fails at connect with manufacturers or stakeholders in general, as intended. The existence of past and current collaborations between many of the potential members of NECTAR, although fragmented, guarantees a low level of risk on the ground of collaborative networking. Also, several partners have a strong connection with instrument manufacturers, software developers, and

end-user stakeholders in industry (e.g. pharmaceutical companies), so that the risk of having no initial connections with stakeholders is low. The members of WG5 will be made aware of the need to maximize the communication and dissemination of NECTAR activities in order to further reduce the level of risk.

3.2 MEASURES TO MAXIMISE IMPACT

3.2.1 KNOWLEDGE CREATION, TRANSFER OF KNOWLEDGE AND CAREER DEVELOPMENT

Meetings, workshops, TSs and STSMs will be employed as vehicles for the sharing, communication and dissemination of top-level knowledge. All the partners will be invited and encouraged to participate and share, as much as possible, new ideas, concepts, techniques and, not less important, new scientific problems and questions, creating strong collaborative working groups. This will be the fundamental way of action that would make NECTAR the perfect way to contribute to an outstanding level of knowledge creation and transfer of knowledge. Become the leading light in this field, NECTAR will act as a pole of attraction for all actors interested in joining an excellent and efficient network, with particular reference to both NNCs and IPCs, both interested in establishing collaborations with European and other NECTAR participants. They will together provide a concrete chance to identify common issues and challenges and to find integrated solutions for researchers whose collaborations are usually limited to a narrow group of scientists (e.g., by geographical, age and/or gender restrictions), thus favouring a better rationalization and harmonization of the available resources. Also, NECTAR will provide a unique opportunity to early-stage and/or talented researchers to acquire new skills and competencies, and to share information on the main challenges in the study of the thermodynamics of chemical transformations. This will support them in developing their independent careers and reaching leadership positions and higher visibility and ensuring that excellence in this field will be continued long after the end of the Action. By exploiting the complementary skills and research fields of various partners, as well as the different nature of involved institutions (e.g., universities, research centres, and enterprises), this network will allow the participants to analyse specific issues in the field of chemical equilibria from very diverse points of view, leading to a global and comprehensive picture of the problem itself. In turn, this will result into an enhancement of the possibility of an integrated approach to its solution, which would be hampered at the level of single groups and without a real networking activity.

3.2.2 PLAN FOR DISSEMINATION AND/OR EXPLOITATION AND DIALOGUE WITH THE GENERAL PUBLIC OR POLICY

The participants in this Action will pursue the aim of strengthening the impact of the study of chemical equilibria in Science through the setup of the largest European community of experts in this field. All the partners will be involved in strong networking activities to share their expertise, facilities, and results within the NECTAR community. Beyond it, communication and dissemination of results and information activities will also take place in order to go beyond its borders. In addition to the audience represented by the potential stakeholders (chemistry research groups, researchers in other scientific disciplines, and industry) we believe that the undergraduate students and the general public are targets of the communication and dissemination activities that need to be taken into account. As for the intra-network communication, the following tools and strategies will be used: i) a dedicated website, which will include a restricted area addressed to information that the consortium needs to leave undisclosed; ii) a database with contact details and description of expertise and facilities of all partners; iii) information on incoming and past meetings, training events and TSs, opportunities for mobility, and the STSMs scheme; iv) a “best practice” area where manuals, protocols and tutorials related to developed methods and instrumentation will be available; v) a list of all publications and presentations resulting from NECTAR activities. Outreach communication and dissemination activities with respect to the consortium will be mainly exploited as follows:

- Emphasis will be placed on making the scientific community aware of the activities of NECTAR. The participation in conferences and workshops (beyond those organised by this Action) will be strongly encouraged. Publication of papers in scientific, peer-reviewed journals will also increase NECTAR visibility to a broader audience of research groups and potential stakeholders, especially in the academia. This will attract not only new partners but also ECIs interested in this topic.

- This Action aims to have, as members, many of the EU leaders in the study of chemical equilibria and, in addition, to attract several non-EU world leaders. With this in mind, communication and dissemination through invited seminars, master/PhD-level courses, summer schools at academic institutions will also take place and will be supported.

- NECTAR members will progressively develop new methods, instrumentation, and software with manufacturers and software companies. The members of this Action will attempt to maximize their participation in trade-fairs, industry exhibitions and forums, in particular with the aim of communicating and disseminating new methods and technology developed within NECTAR.

- NECTAR members will pursuit the communication and dissemination outside the scientific community. As examples, the researchers will be strongly encouraged to present NECTAR activities at events for citizens, open-days at universities, presentations at schools. The research groups at universities will also involve undergraduate students in the NECTAR activities, offering them a unique opportunity to carry out their undergraduate research in an international environment, and in collaboration with world leaders in the area of the study of chemical equilibria.

4 IMPLEMENTATION

4.1 COHERENCE AND EFFECTIVENESS OF THE WORK PLAN

4.1.1 DESCRIPTION OF WORKING GROUPS, TASKS AND ACTIVITIES

The NECTAR Action will be initially composed by five WGs. Participants of the WGs will be researchers with different skills to promote the build-up of an interdisciplinary working environment. This will be of paramount importance for the exchange of knowledge within, and outside, the academic community, in particular toward external subjects and stakeholders (e.g., industries, public administration). Of the five WGs, three will be *objective-oriented* (WGs 1-3), one *service-oriented* (WG4) and one *communication and dissemination-oriented* (WG5). These five WGs will guarantee a high efficiency in project development since the beginning of the project. In particular, the activities within WGs 1-3, will exploit an adequate national and international research funding and a strong partnership between all members of each WG. In this respect the past and current collaborations between some of the COST participants will be the basis for a quick implementation of the activities in WGs 1-3. Furthermore, in agreement with NECTAR general objectives the networking will be established and managed through a straight cross-collaboration between all WGs. Tight interconnections between the WGs scientific programs will be pursued on transversal objectives such as systems under investigation, procedures, or computational approaches. In this respect, the participation in more than one WG will be also promoted. WG4 will provide the participants with: i) the design, synthesis and characterization of new molecules, supramolecular systems and/or chemical devices for specific needs; ii) computational tools for the study of chemical equilibria; iii) guidelines and protocols for best performance in designing and carrying out experiments; iv) assistance in modelling systems investigated by WGs 1-3. WG 4 will therefore be not focused on specific systems, but its activities will complement those of WGs 1-3. When mastered, they will enhance the performances of fundamental research and applications and will be beneficial not only for other WGs, but also for the scientific community outside this project. The success of the Action also hinges on the outreach and dissemination activities, thus a specific WG will be implemented (WG5). This WG will be specifically focused in planning and keeping track on outreach, communication and dissemination activities. Among the activities of this WG, fully listed below, there will be web-based and media communication. The group will not only target the NECTAR community, but also external collaborators, industries and global audience and stakeholders in general. This will foster the collaboration between research groups and industry, which is essential for the development of new chemical systems, procedures, technologies and applications. As a whole and on a mid-long term, WGs activities will pursue the general NECTAR aims and objectives. NECTAR WGs will however consider short term objectives that will be progressively fulfilled in the timeframe of the Action. The attempt to quickly tackle and solve the problems listed in section 1.1.2 is the urgent goal of this Action: in this light, main (but not limited) tasks and activities planned within single WGs are presented below.

WG1 – NECTAR for highly hydrolysable (HHC) and/or low-valence state (LVC) cations

Rationale: Equilibrium analysis of systems containing highly hydrolysable or low-valence state cations is always very challenging. Typical bottlenecks are difficult experimental set-up (e.g., formation of sparingly soluble species for HHC, oxidation for LVC in the presence of traces of dioxygen or other oxidants, etc.), lack of reliable literature data (e.g., unreliable speciation models, missing and/or questionable thermodynamic parameters, literature discrepancies, etc.), or narrow ranges of experimental conditions explored to date (e.g., temperature, ionic media and ionic strengths, presence of competing ligands, etc.), that are inadequate for the interpretation of phenomena at specific conditions.

Tasks: Defining precise strategies for the study in solution of systems containing HHC (e.g., Zr(IV), lanthanoids, actinoids, oxoions). Defining procedures and experimental approaches for the study of LVC (e.g., Fe(II), Sn(II), Cu(I)), especially those spectroscopically silent (e.g. Cu(I)). Providing protocols for the study of the speciation of HHC and LVC under conditions of interest for biological, environmental and technologically/industrial applications. Providing reliable, accurate and comprehensive sets of thermodynamic data of systems containing HHC and LVC in a wide range of different experimental conditions.

Activities: Determination of the hydrolysis constants (and other thermodynamic parameters) of HHC and LVC. Study of complexes of HHC and LVC: speciation, solubility, kinetics of formation, redox properties. Structural study and correlation of structural information of the complexes with solution properties. Modelling of the speciation of the complexes as a function of different conditions (e.g., total cation concentration, pH, pe, ionic strength, system composition, temperature). Validation of data through interlaboratory and blind round-robin experiments to check reliability and consistency of results obtained. Dissemination of results, especially those related with experimental procedures.

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

Rationale: Strong binding of metal ions (sequestration) and selectivity of binding are processes of outmost importance for several applications (e.g., chelation therapy, nuclear medicine, environmental remediation, metal recovery, water treatment). Strong binding can be operated by a large number of ligands (natural or synthetic) which all share the property of forming very stable complexes. The determination of corresponding thermodynamic equilibrium data is extremely difficult, and cannot be performed by classical approaches. In addition, complexes of some pre-organised ligands (e.g. those currently used in medicine) are formed very slowly, and kinetical aspects have to be considered to get correct thermodynamic data. Also, similar ligands which have limited structural differences often form complexes with the same metal ion that differ in stability by orders of magnitude. Therefore, the design of selective ligands requires a precise knowledge of structure-stability relationships.

Tasks: Defining recommended experimental procedures and guidelines for the accurate determination of stability constants and other thermodynamic parameters for systems involving natural and synthetic strong chelators, macromolecules, and polyelectrolytes. Exploring rational or combinatorial strategies, supported by *in silico* studies, for the design of new ligands for the selective recognition of metal ions or small molecules in solution.

Activities: Evaluation of the sequestering ability and selectivity of existing and new chelating agents that are of current interest for the scientific community or for the stakeholders (e.g., metallophores, new-generation complexones, etc.) Study of the speciation of systems containing structurally complex (macro)molecules (e.g., nucleic acids, peptides and proteins, organic matter, polyelectrolytes). Cross-evaluation of methods for the study of the thermodynamic selectivity. Setup of protocols and guidelines for the study of these systems and the determination of their thermodynamic parameters. Formulation of user-friendly strategies for data analysis, and their dissemination.

WG3 – NECTAR for multicomponent solutions and complex matrices

Rationale: Thermodynamic and chemical equilibrium data are nowadays needed for the most diverse applications, including speciation studies of real systems (e.g., natural waters, biological fluids, commercial products). Classical procedures for the study of the equilibria in solution are often inadequate when a high number of components is present in the system. For these reasons, the investigation of multi-component systems or systems in complex matrices (e.g. ionic liquids, mixed solvents, heterogeneous systems, etc.) is becoming challenging. In this respect, there is an urgent need to update and adapt experimental procedures and computational approaches.

Tasks: Defining recommended experimental and data analysis procedures and guidelines for an accurate speciation of systems with multiple components. Defining recommended experimental and data analysis procedures and guidelines for an accurate speciation of systems in complex matrices such as ionic liquids, mixed solvents, systems containing surfactants or sorbent materials.

Activities: Determination of the stability constants (and other thermodynamic parameters) of weak complexes. Evaluation of the network of interactions of the medium components. Setup of reliable speciation models of real systems. Characterisation of ternary (or higher) species and experimental determination of their stability. Determination of speciation models for surfactants. Setup of new accurate models for speciation studies in ionic liquids and mixed solvents. Standardisation of protocols for the experimental determination and data analysis for heterogeneous systems containing strong sorbent materials.

WG4 – NECTAR tools, services and facilities

Rationale: Fundamental research and applications of chemical thermodynamics require a series of *tools*, *services* and *facilities*, whose availability is of paramount importance. For instance, *specific* ligands/molecules and/or chemical devices with *specific* characteristics and properties are needed in *specific* contexts, while dedicated software (e.g., for experimental data treatment, speciation models, molecular models and theoretical calculations) is required for the determination of thermodynamic parameters. Associated to the latter problem, non-experts in the field need guidelines for the experimental determination of thermodynamic parameters and their analysis, especially for the less conventional types of experiments. Finally, it will be desirable for the entire scientific community to have a comprehensive database for the deposition and retrieval of reliable thermodynamic parameters.

Tasks: Providing molecules and chemical devices for specific purposes. Providing updated guidelines, software and services to enhance the performances of both research and applications in equilibrium thermodynamics. Studying molecular models by theoretical calculations and the correlation between the calculated stability and experimental thermodynamic parameters.

Activities: Design, synthesis and characterization of new molecules, supramolecular systems or chemical devices for specific needs. Optimisation and setup of 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. Development of 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).

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

Rationale: Scarce information and lack of communication or dissemination represent, beyond any doubts, a bottleneck for the advancement of knowledge. This is valid not only within a well-defined community of scientists such as that of a COST action. In science in general it often happens that research is performed ignoring the fact that a method, technology, or result obtained in a specific context can be extremely relevant also from the perspective of other scientific areas. Furthermore, intersectoral research projects and training schemes need to be established in the future. At least at European level NECTAR aims to promote the communication between all subjects (from academia to stakeholders) favouring, in turn, the implementation of intersectoral collaborations. In the long term we believe that this will address societal and economical needs.

Tasks: Organisation of meetings to favour contacts between research groups. Coordination of STSM plans. Design and management of Action website. Coordination of activities aimed at starting new research projects. Promotion and help the network members to apply for competitive European funds and other international research and innovation grants. Contacts and partnerships with stakeholders to increase academia-industry interactions, valuable for innovative ideas and discoveries, to maximise protection of intellectual property rights and commercialization of products of the research.

Activities: Organisation of COST Action networking events (meetings, TSs, STSMs). Coordination and promotion of ITCs participation (increasing the number of partners), as well as the participation of the non-academic organisations. Contact with industrial partners will help to understand "how could

science meet business", and the mechanisms and perceptivity of business implementations of innovative scientific ideas. Organisation of joint scientific publications and formation of multidisciplinary research consortia. Organisation of project-writing seminars. Development of documents with aims, directions, and strategies for future research. Provision of up to date information on funding opportunities. Organisation of entrepreneurship workshops and seminars. Attraction of further world experts. Implementation of the Action website. Monitor the whole Action activities to assure gender balance.

4.1.2 DESCRIPTION OF DELIVERABLES AND TIMEFRAME

We ambitiously expect to generate top quality foreground knowledge as well as training of human resources through NECTAR. Immediate deliverables are represented by the identification of the main specific problems tackled by the *objective-* (WGs 1-3) and *service-oriented* (WG4) groups, that will turn into a plan of the activities of the WGs. Main deliverables expected from these WGs can be summarised as follows: elaboration of annual reports to present to the MC; reports of STSMs, supporting/teaching material for TSs (with WG5); publication of internal reports, reports and guidelines for the scientific community, high-level scientific research articles/reviews in peer-reviewed scientific journals; publication of relevant findings on Action website and in general and professional social media (with WG5); registration of patents; elaboration and publication of workflows, new protocols and guidelines; new/upgraded databases; new software; new instruments and/or interfaces; training and delivery of early stage researchers through the planned actions; submission of joint research projects; intensification of relationships and promotion of chemical thermodynamics with stakeholders and institutions; outreach activities oriented to the general audience. Furthermore, specific milestones and deliverables will be attained by WG5: Action website; submission of research projects; flyers and brochures to present the Action; publication of relevant findings on Action website and in general and professional social media; reports on annual Action meetings; TSs (min. 1 / year); STSMs (min. 10 / year); report of final Action meeting. Among others, the number of papers published in collaboration between NECTAR groups over 4 years (more than 20% of the total published by the participants in the field of chemical equilibria), the number of participants attending to the WG meetings and TSs (> 30% per meeting) and the number of international/multilateral projects presented and/or the number of patents registered (> 1 / year) will be considered as further indices of the success of NECTAR.

At the very beginning of NECTAR activity, a kick-off meeting of the Action will take place. This meeting will be crucial to define coordination and strategy details of the Action, as well as to discuss and approve several guidelines, in particular those related to the participation, open-access policy and associated funds, confidentiality, and intellectual property. Afterwards, the MC will meet at least yearly to coordinate all Action activities. In addition to the MC, a Core Group (CG) will be also created in support of the MC, which will directly report to it. The CG will coordinate and supervise the technical/scientific activities of the Action. Its role will be to steer and monitor the Action as approved by the MC and would be tasked with responding efficiently to issues requiring urgent input and/or decision-making. The CG will comprise the Action Chair, Vice-Chair(s), the WG Leaders, the Grant Holder, a Training Schools Coordinator (TSC, responsible for organising the TS), an STSM Coordinator (STSMC, that will organise and manage STSMs), a Dissemination Manager (DM, responsible for organising the communication and dissemination policy of the Action, seeking opportunities to address all groups of collaborators), an Industry Transfer Manager (ITM, for advertising and promoting results and activities of the action at stakeholders, and for organising meetings with industrial partners), and an Equal Opportunities Manager (EOM, responsible for fulfilling the requirements of gender balance, involvement of ECIs and ITCs). The CG will meet regularly at least twice per year, one preferably in concurrence with the MC meetings to reduce costs. WG Leaders will be responsible for the organisation and coordination of the WG meetings. WG leaders will also hold the responsibility of the effective WG activities, deliverables, and report to CG and MC. WG objectives and tasks will be revised and upgraded periodically. TSs will be organised preferentially by two or more WGs, to provide opportunities for ECIs to gain new skills and build a new generation of researchers with broad expertise. The program of TSs will be advertised on the Action website, on mailing lists. The results of STSMs will be presented at WG meetings, and summarised on the website (where possible for Intellectual property rights). TSC and STSMC will operate in close contact with WG Leaders. The DM will manage a dedicated calendar of events and conferences attractive to the Action and to find a significant number of participants that can represent NECTAR at those events. The DM will also be responsible for communicating and disseminating the Action goals as well as its progress toward the objectives at different subjects (academia to stakeholders). For these reasons the activities of the DM will be strongly linked with the ITM, aiming at efficient entrepreneurship.

A plenary meeting of all the members of the Action will be organised once a year in different countries. Besides scientific sessions, one session will be dedicated to the presentation and discussion of the Action's progress as well as of the results, deliverables and milestones. All the outputs will be reviewed and the forward strategies for the Action will be discussed. A final meeting will be organised in the format of a scientific conference. The participation of groups from other COST Actions which are interested in chemical thermodynamics will be encouraged. The initial management structure described here above is designed on the size of NECTAR network based on the current number of proposers. Changes in the structure, if required by a significant change in the size of the Action in terms of participant, will be proposed in due course. A detailed picture of the Action timeframe in the current design is shown in Gantt diagram below.

4.1.3 RISK ANALYSIS AND CONTINGENCY PLANS

The great enthusiasm and willingness to collaborate shown by all the proposers during the preparation of NECTAR Action is already an excellent indicator for the success of this Action. Furthermore, the internationally recognized experience and know-how of all the research groups involved minimize the risks of failure on the scientific achievements proposed. Many of the research groups and institutions who expressed their interest in joining this Action have already collaborated in the past, albeit in small clusters. Despite these already established contacts, unexpected problems on the ground of collaboration may arise during the course of the Action. If such situations arise, several actions would be immediately taken, mainly by the MC, which has the responsibility of assessing the progress of the Action regularly, and taking corrective and incentive measures to ensure the success of NECTAR network. Some of the potential risks for the success of the Action and the corresponding contingency actions are listed below:

Network expansion failure (scale and/or impact), in particular toward the private sector. To tackle this possible issue, constant monitoring of the communication and dissemination plan will be carried out. This will enable actions such as improving identified weak communication channels, enhancing communication and dissemination capacity to be executed. Implementation of new and stronger links to relevant EU and national authorities may also cut this risk.

Low number of ECIs and/or weak gender balance. Organising more attractive STSMs and TSs will spur good participation and involvement of ECIs in the Action activities. The enrolment of ECIs on leadership positions would be also a good incentive. Providing childcare options during Action events as STSMs or TSs, especially when this is a hindrance in terms of gender balance participation, will be important as well. The activities of the EOM will be principally oriented in minimizing this risk.

Low involvement of the partners and low outcomes. Increasing the number and the diversity of activities aiming at growing interest toward the action: additional seminars, conferences, workshops.

4.1.4 GANTT DIAGRAM