SHORT TERM SCIENTIFIC MISSION (STSM)
SCIENTIFIC REPORT

This report is submitted for approval by the STSM applicant to the STSM coordinator

Action number: 18202 Network for Equilibria and Chemical Thermodynamics Advanced Research

STSM title: Development Thermodynamical data sets

STSM start and end date: 16.09.2022 to 30.09.2022

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PURPOSE OF THE STSM:

The purpose of the STSM is to perform structure-thermodynamics correlation analysis based on the crystallographic data deposited in Cambridge Crystallography Database (CCDC) that relate to structures of particular families of compounds that exerts different properties. In addition, partially to utilize the published crystallographic data (e.g. non-covalent bond energies/ bond distances, mainly different types of H-bonds) as a models for developing case studies with encompass the appropriate data sets that might be used for developing the algorithmams for particular applications in calculation the possible non-covalent interactions in molecular crystals.

DESCRIPTION OF WORK CARRIED OUT DURING THE STSMS

The working plan was carried out toward the following activities:

- Crystal structures searches in CSD (Cambridge Crystal Structure Database) for the structures of groups of compounds, some of which previously I was used for experimental screening protocols for cocrystallizing multicomponent crystals (molecular salts and cocrystals), and determination of their structures by single-crystal X-day Diffractometry.
- Statistical analyses of each compound model for the frequency of appearing of its crystal structures in form of monocomponents single phases (e.g. polymorphs or organo-metallic compounds) or as singe phase multicompnent crystals (salts, cocrystals or hydrates/solvates and their polymorphs)
- Statistical analyses of the prevalence of occurring the particular non-covalent type of interactions (e.g. Charge-assisted H-bonds, Resonance stabilized H-bond etc.) for each of the model compounds which is structure form multicomponent crystals.
- Statistical analyses of the H-bond's type/ geometry of motifs (e.g. dimmers, trimers, tetramers, catamers homomeric and/or heteromeric synthons) in crystal structures.
- Using a Mercury program (part of CSD) for measuring the bond distances and angles, angles between the planes and torsion angle for packed molecules into crystal structures
- Onsite visiting the laboratory facilities for carrying out research on mechanochemical processing/ synthesis of multicomponent crystals and solid-state reaction (e.g. ball mills with different design

and capacities)
- Onsite visit of the laboratory facilities for solid-state characterization (X-ray diffractometars, Thermal analyses, Spectroscopy)
- Attending appointments discussing the opportunities for mutual collaboration on crystal structures determination and solid-sate reaction and cocrystallization by utilizing mechanochemistry.

DESCRIPTION OF THE MAIN RESULTS OBTAINED

Searching engine approach by drowing molecular structural moieties for specific group of compounds (e.g. guanide, biguanides, enediol group of organic small size compounds and ect.) offered selection of the collections/ clusters of structures deposited in CSD (Cambridge Structure Databese) and for each structure reliable crystallographic parameters (e.g. nature of noncovalent interactions, bond distances, bind angle, torsion angle and ect.) that offer the opportunity to develop thermodynamic (TD) models for TD properties of the multicomponent crystalline phases, and thus to get insight in structure-properties relationship. The feasible thermodynamic model must be based on an understanding of the known crystal structure of a phase, e.g., the number of sublattices, and the occupation of molecules on the crystallographic sites. The energies and intermolecular interactions occurring within the crystals were explored, applying crystal lattice energy calculations and Hirshfeld surface analysis Some simplification is however sometimes necessary to minimise the number of parameters necessary to describe the thermodynamics of a phase. Theoretical models, such are calculations based on Density Functional Theory (DFT) assuming vapour or liquid phases, as well the semi-empirical (statistically significant dataset for crystallographic parametars) provide an invaluable tools by calculating the energies of different crystallographic configurations to identify which features are key to guide such simplification. These models are employed to calculate the enthalpies of the formation, crystal structure and energies associated with defect formation and the solution of additional elements onto the crystal lattice.

FUTURE COLLABORATIONS (if applicable)

The follow-up activities address the expectation to be established based on the mutual research collaboration (e.g. jointly application for mutual research projects or being project''s partner) in frame of which jointly publications would be issued, participation to scientific events (workshops, conferences, fairs etc.), thus obtaining the dissemination of the accomplished research toward the scientific community.

Promotion of the COST CA 18202 Network for Equilibria and Chemical Thermodynamics Advanced Research (NECTAR) toward the highlighting of NECTAR logo on the poster and acknowledge the NECTAR in the published paper, hence promotiong the NECTAR mission toward the scientific community.

Based on the recent literature survey the drafted text for part of manuscript (Introductiry part) was prepared and submitted to the WG4 NECTAR's peers for developing review type of publication that tackle utilizing the Thermodynamic parameters for developing reliable algorithams for particular applications.