

Czochralski Advanced Crystal Engineering Laboratory (aceLAB)



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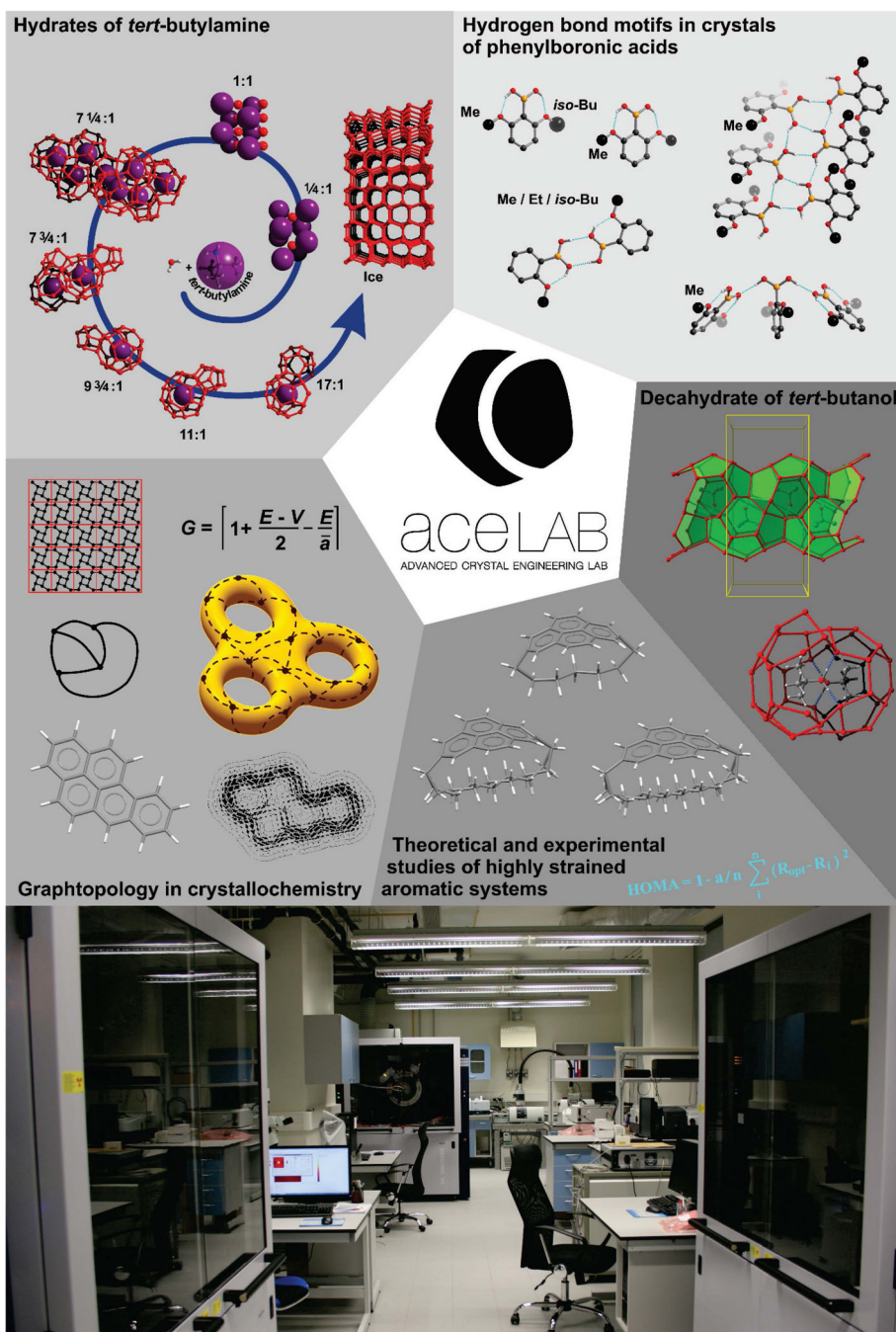
RESEARCH PROFILE:

Our scientific interest covers a broad spectrum of problems in structural chemistry of small organic compounds, physical organic chemistry, chemical crystallography, crystal engineering and forensic science as well.

The research includes both theoretical investigations of such topics as aromaticity, substituent effect in chemistry, solvent effect and experimental studies on crystallization and crystal structure analysis including polymorphism, phase transitions, twinning, disorder, stability of molecular crystals. The experimental part is supported by molecular modeling including quantum-mechanical calculations (ab initio). To explain some fundamental problems in organic chemistry we also introduce and apply new theoretical approaches based on graph topology. In our research we use the following experimental techniques: single crystal X-ray diffraction, in wide range of temperatures (including room temperature high pressure investigations) combined with Raman spectroscopy; powder diffraction; calorimetric measurements (DSC, TGA/DSC). To devise and obtain novel crystal structures a world-unique IR laser supported in situ crystallization device is applied. Our particular interest is also focused on development of new methodologies and research equipment.

CURRENT RESEARCH ACTIVITIES:

The experimental part is primarily related to the design and physicochemical characterization of new crystalline hydrates/hydrate clathrates of small organic compounds, that are liquids at room temperature. To elaborate intermolecular interactions in the solid state, to create novel architectures, many other multi-component systems, such as supramolecular complexes of phenylboronic acids, benzenoid hydrocarbons or a clathrate-like systems formed by urea, are also investigated. The primary theoretical topics of our investigations include: relation between strain and aromaticity, energetic aspects of cyclic π -electron delocalization, definition of aromaticity, comprehensive physicochemical interpretation of substituent effect, dependence between the strength and the nature of hydrogen bond and π -electron delocalization in model systems of biological importance. Our Laboratory is equipped with two single crystal and one powder X-ray diffractometers, Raman spectrometer, DSC and TGA/DSC instruments.



SELECTED PUBLICATIONS:

1. A. Rękorajska, G. Cichowicz, M.K. Cyrański, M. Grdeń, M. Pękała, G.J. Blanchard, P. Krysiński, Synthesis and Characterization of Tb-Doped Nanoferrites, *ChemNanoMat*. 4 (2018) 231-242.
2. D. Basiak, T. Wojciechowski, A. Plichta, Z. Ochal, P. Socha, P. Rzepiński, Ł. Dobrzycki, W. Ziemkowska, Chiral dialkylaluminum 6,7-dihydro-5H-pyrrolo[1,2-a]imidazol-7-olates: Synthesis, characterization and polymerization activity, *Journal of Organometallic Chemistry*. 848 (2017) 302–308.
3. S.E. Kutyla, D.K. Stępień, K.N. Jarzemska, R. Kamiński, Ł. Dobrzycki, A. Ciesielski, R. Boese, J. Młochowski, M.K. Cyrański, Structural and Stability Studies of a Series of para-Phenylenediboronic and para-Hydroxyphenylboronic Acid Cocrystals with Selected Aromatic N-Oxides, *Crystal Growth&Design*. 16 (2016) 7037–7050.
4. Ł. Dobrzycki, K. Pruszkowska, R. Boese, M.K. Cyrański, Hydrates of Cyclobutylamine: Modifications of Gas Clathrate Types sI and sH, *Crystal Growth&Design*. 16 (2016) 2717–2725.
5. Ł. Dobrzycki, P. Taraszewska, R. Boese, M.K. Cyrański, S.A. Cirkel, Towards Clathrates: Frozen States of Hydration of tert-Butylamine, *Angewandte Chemie-International Edition*. 54 (2015) 10138–10144.
6. M.A. Dobrowolski, G. Garbarino, M. Mezouar, A. Ciesielski, M.K. Cyrański, *CrystEngComm*. 16 (2014) 415–429.
7. A. Ciesielski, T.M. Krygowski, M.K. Cyrański, A.T. Balaban, Defining Rules of Aromaticity: a Unified Approach to the Hückel, Clar and Randić Concepts, *Physical Chemistry Chemical Physics*. 13 (2011) 3737–3747.
8. M.A. Dobrowolski, M.K. Cyrański, B.L. Merner, G.J. Bodwell, J.I. Wu, P.v.R. Schleyer, Interplay of π -Electron Delocalization and Strain in [n](2,7)Pyrenophanes, *Journal of Organic Chemistry*. 73 (2008) 8001–8009.
9. M.K. Cyrański, T.M. Krygowski, A.R. Katritzky, P.v.R. Schleyer, To What Extent Can Aromaticity Be Defined Uniquely?, *Journal of Organic Chemistry*. 67 (2002) 1333–1338.
10. T.M. Krygowski, M.K. Cyrański, Structural Aspects of Aromaticity, *Chemical Reviews*. 101 (2001) 1385–1419.