

## Poster Presentation

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### *Coordination modes of novel 4,5-dicyanoimidazolato ligand in alkali metal salts*

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As the use of lithium batteries became more and more wide-spread, the importance of the research on novel salts for batteries' electrolytes grew more and more important. The focus has been put on designing novel lithium and sodium salts which dissociate well in aprotic solvents and are electrochemically and thermally stable. Salts with heteroaromatic anions such as 2-trifluoromethane-4,5-dicyanoimidazolate (LiTDI) [1,2] are a promising alternative for the salts commonly used as charge carriers in lithium and sodium batteries. The class of new 4,5-dicyanoimidazolates ligands is based on N-heterocyclic five-membered ring substituted with nitrile group. Such a type of anions possesses four nitrogen donor centers able to coordinate cation, and is characterized by charge delocalization, both on imidazole ring and cyano substituents resulting in extended  $\pi$  electron system. In solid as well as liquid electrolytes one should expect the co-existence of a variety of ionic species, such as isolated anions and cations solvated by solvent molecules, ionic pairs, for which the coordination sphere of cations is completed with solvent molecules, as well as dimers and aggregates with varied stoichiometry. The observed degree of aggregation depends mostly on the coordination properties of anions, their ability to form hydrogen bonds and their compatibility with the acidic properties of cations. The increase of the salt concentration should result in association process and the emergence of higher aggregates, up to polymeric systems, possessing structure of chains, ribbons, layers or networks. In order to define the coordination ability of the class of new ligands, we examined their organization modes in the alkali metal salts and have found a wide variety of mentioned motifs. Discovering and understanding the phenomena related to the organization of such systems in the solid state is crucial for the elaboration of novel electrolytes and should give information about cation and anion coordination in electrolytes. Our single-crystal diffraction studies have shown that new salts comprising 4,5-dicyano-2-(trifluoromethyl)imidazolato anion are interesting from the point of view of their crystalline structure, offering variety of possible coordination modes and are, therefore, worthy of examination.

[1] L. Niedzicki, G.Z. Zukowska, M. Bukowska, et al, *Electrochimica Acta*, 2010, 55, 1450., [2] M. Dranka, L. Niedzicki, M. Kasprzyk, et al, *Polyhedron*, 2013, 51, 111.

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