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Engineering Phase Change Behaviours of Organic Ionic Plastic Crystals for Development of Solid State Electrolytes

Plastic Crystals are materials in which the molecules or ions occupy the same center of mass as in regular crystal lattice but have freedom of rotation. They show typical disorder-order transitions that lead to realize various sort of functional materials. Especially, organic ionic plastic crystals (OIPCS) have gained much attention over the past years thanks to their potential usage as solid-state electrolytes [1, 2].
The aim of this work is basically twofold. Firstly, we are interested in investigating the counter-anion dependence of the plastic phase transitions in a series of R-(+)-(3)-hydroxyquinuclidinium salts [QH]X. By varying size, shape, and charge of the anion, we expect to obtain different behaviors in terms of plastic phase transition and type. Second, we want to explore the possibility of preparing crystalline solid solutions, studying how the composition of the resulting materials further affects the phase transition compared to the pure parent systems.
To that end, we synthesize a series of [QH]X salts with various counter-anions, including the tetrahedral anions sulfate (SO42−), tetraphenylborate (BPh4−), tetrafluoroborate (BF4−), and the octahedral hexafluorophosphate (PF6−) by the metathesis of [QH]Cl using metal salts of the corresponding anions. A combination of solid-state techniques, including variable temperature XRD, thermal analyses, multinuclear (11B, 13C, 15N, 19F and 31P) solid-state NMR spectroscopy, variable temperature wideline 19F T1 relaxation measurements and micro-Raman spectroscopy are used to elucidate crystal structures and phase transition behavior of the so-obtained materials. The figure below shows the structural outcomes of one of the compound we are working on quiniclidinol hexafluorophosphate [QH]PF6 [3].

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