

Ionic Conductivity and Electrochemical Properties of Lithium Orthoborate Salts

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Lithium salt plays an important role in lithium and lithium ion rechargeable batteries. Many kinds of new lithium salts have been synthesized and studied in recent years [1-8]. One of them is lithium salt of chelated orthoborate. It has been reported that these orthoborate salts have very good ionic conductivity and wide electrochemical stability in solutions [7,8].

In our recent publications [9,10] we reported that the orthoborate salts based on perfluoropinacol and dicarboxylic acids, have extremely high ionic conductivity and good electrochemical stability in solutions. The high conductivity is due mainly to the unusually weakly coordinating anions.

In the present work, we compare the physical properties and conductivities of three of the new lithium orthoborate salts. The three lithium salts are lithium bis(perfluoropinacolato)borate (LiBPFPB), lithium bis(oxalato)borate (LiBOB) and lithium bis(malonato)borate (LiBMB). Computational molecular mechanics models of the three orthoborate anions show that the oxygens in BPFPB⁻ anion are least exposed. The oxygens bonded to boron are slightly less negative in BOB⁻. The BMB⁻ anion has four lowest energy conformers. The glass transition temperature (T_g) of LiBPFPB and LiBOB cannot be measured directly, but the extrapolation of LiBPFPB-PC binary system shows LiBPFPB has a low T_g at around -37°C .

These three lithium salts show very high ionic conductivities in solutions. The conductivity is nearly independent of the salt content in the salt concentration range of 0.5 ~ 1M, which is advantageous for their applications.

Electrochemical stability of LiBOB measured in the oxidation-resistant solvent ethyl methyl sulfone (EMS) [11] using different electrodes, is comparable to that of LiPF₆ — the present lithium battery industry standard.

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