Lithium imidazolide (LiTDI) as a challenger for LiPF$_6$ in lithium batteries

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Lithium salts having an Hückel anion derived from imidazole such as lithium 4,5-dicyano-2-(trifluoromethyl) imidazolide (LiTDI) have been synthetic in 2008 by Leszek Niedzicki et Michel Armand and a patent has been deposited in 2009 [1,2]. Among all imidazole derived salts, LiTDI is probably the most promising and could be a challenger to LiPF$_6$ in the future. Unlike to LiPF$_6$, this salt is not water sensitive and stable at high temperatures (200°C). As no HF is expected to be produced during battery cycling, corrosion of cathode material or metallic collector is avoided. LiTDI solutions in alkylcarbonate (AC) are able to form an adequate passivation layer on graphite and are compatible with high voltage cathodes up to 4.7V. Like LiPF$_6$, LiTDI based electrolytes are able to passivate aluminium collectors. The main drawback of LiTDI is the lower conductivity (6.8 mS.cm$^{-1}$ à 1 mol.L$^{-1}$ in EC/DMC à 25°C, Niedzicki et al.) as compared to LiPF$_6$ in the same AC solvent mixtures.

![Structure of the TDI Hückel anion](image)

In this work LiTDI is compared to competing salts like LiTFSI, LiFAP and LiPF$_6$ in a EC/DMC (50/50 wt%) mixture. Transport properties such as viscosity, Li$^+$ and anion diffusivity and lithium transference number, were investigated and show the inadequacy of the EC/DMC mixture as only 36% of the ion-pairs are dissociated.

Taking into account these results, a new solvent mixture (quoted as NSM in the following) has been designed. The LiTDI/NSM electrolyte has been tested and compared to the LiPF$_6$/AC electrolyte in graphite (GR) and NMC half cells at different rates of discharge.

All results confirm that LiTDI/NSM could replace LiPF$_6$ as an electrolyte in many Li-ion batteries.