An insight into coordination ability of dicyanoimidazolato anions toward lithium in presence of acetonitrile. Crystal structures of novel lithium battery electrolyte salts.

Maciej Dranka*, Leszek Niedzicki, Marta Kasprzyk, Marek Marcinek, Władysław Wieczorek, and Janusz Zachara

Department of Chemistry, Warsaw University of Technology, Noakowskiego 3, 00−664 Warsaw, Poland

Supporting Information

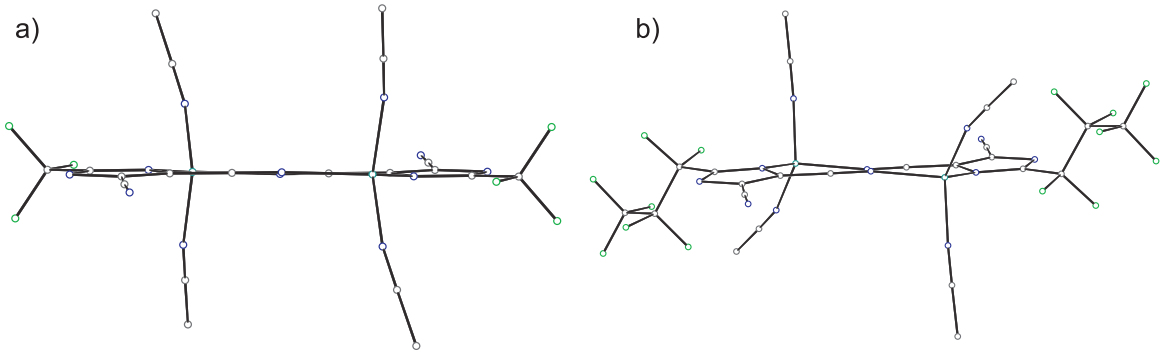

Figure S.1. The planarity of the central ring in a) **1** and b) **3**.

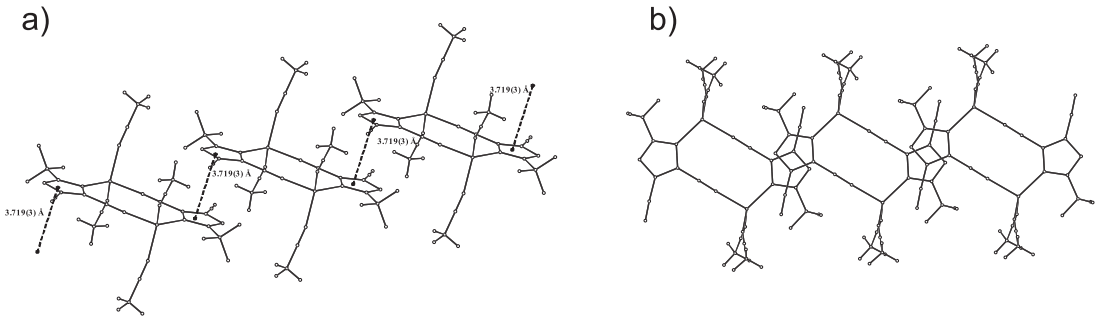

Figure S.2. Depiction of a) centroid-centroid distance and b) shift displacement (view along normal to imidazole ring) between two imidazole rings showing π-π interaction.

Table S.1. π-π contacts in **1**−**3**.

Distance/Å	**1**	**2**	**3**
centroid-to-plane	3.530(3)	3.662(2)	3.697(2)
centroid-to-centroid	3.719(3)	3.788(2)	3.845(2)
shift displacement	1.170(3)	0.968(2)	1.057(2)