

# Characterization and quantification of LiPF<sub>6</sub> extracted from lithium-ion batteries via heteronuclear NMR and ERETIC software

S. Ghezzi,<sup>‡</sup> D. Maggioni<sup>†</sup>, M. Magni<sup>‡</sup>

<sup>‡</sup> Department of Environmental Science and Policy, Università degli Studi di Milano, via Golgi 19, 20133 Milano (Italy) E-mail: simone.ghezzi1@unimi.it

<sup>†</sup> Department of Chemistry, Università degli Studi di Milano, via Golgi 19, 20133 Milano (Italy)

The growing volume of electronic waste (e-waste), particularly end-of-life (EoL) lithium-ion batteries (LIBs), poses significant environmental challenges. With EU regulations aiming for ambitious recovery rates of critical metals, such as lithium, by 2030–2031 [1], the need for efficient, scalable, and environmentally friendly recycling methods of these devices is urgent.

LiPF<sub>6</sub> is currently the most used lithium salt for LIBs as an electrolyte, but it has various drawbacks regarding its stability, which usually contributes to the aging and eventually failing of the battery [2].

The first part of this presentation will be focused on a study about <sup>31</sup>P and <sup>19</sup>F NMR spectra executed on LiPF<sub>6</sub> to characterize its decomposition byproducts.

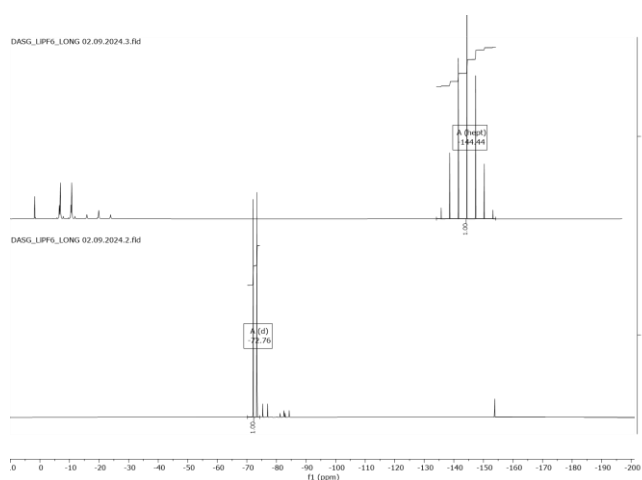


Fig. 1. <sup>31</sup>P (up) and <sup>19</sup>F (down) NMR spectra from a LiPF<sub>6</sub> decomposition experiment (time = 40 days)

The second part of the presentation will go in the details about how <sup>31</sup>P NMR coupled with the ERETIC software [3] can be used to quantify the lithium salt extracted from LIB scraps.

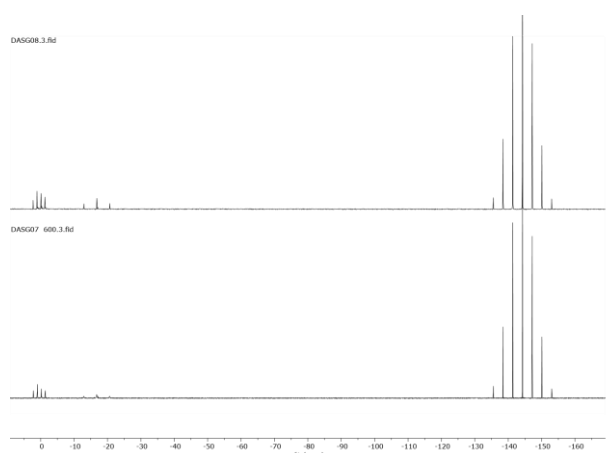


Fig. 2. <sup>31</sup>P NMR spectra of two samples of LiPF<sub>6</sub> extracted from spent LIBs, exhibiting different degree of decomposition

## Referenze

[1] European Parliament, *Official Journal of the European Union L 191*, 28.7.2023, 1-117, ELI:

<http://data.europa.eu/eli/reg/2023/1542/oj>

[2] B. Vortmann, S. Nowak, and C. Engelhard, *Analytical Chemistry* 85(6), 3433-3438 (2013)

[3] L. Barantin, A. Le Pape, and S. Akoka, *Magnetic Resonance in Medicine* 38(2), 179-182 (2005)