Molecularly Tuned 4-Phosphoryl Pyrazolones for Lithium Recovery and Selective Rare Earth Extraction

Dr. Jan J. Weigand

Faculty of Chemistry and Food Chemistry, Technische Universität Dresden, 01069 Dresden, Germany
E-mail: jan.weigand@tu-dresden.de

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Resumen

The sustainable recovery of lithium and related strategic metals is a key challenge in energy transition technologies. Herein, we present a structurally guided approach using 4-phosphoryl pyrazolone ligands in pH-controlled liquid-liquid extraction (LLE) systems. These ligands enable highly selective separation of lithium from coexisting alkali and alkaline earth elements such as Na^+, K^+, Mg^{2+}, and Ca^{2+}, achieving extraction efficiencies of up to 94% under optimized conditions. In-depth NMR, MS, and SC-XRD studies reveal the formation of di- and trinuclear lithium complexes that correlate with extraction performance. Co-ligand effects, especially from trioctylphosphine oxide (TOPO), were systematically evaluated to enhance metal-ligand interactions and tune selectivity. Beyond lithium, preliminary results demonstrate that structural modifications to the pyrazolone scaffold allow controlled interaction with rare earth elements (REEs), highlighting the potential of this ligand platform for broader separation applications. This work provides mechanistic and structural insight into alkali-REE separation and opens a pathway toward ligand-tailored, greener extraction systems.

References:

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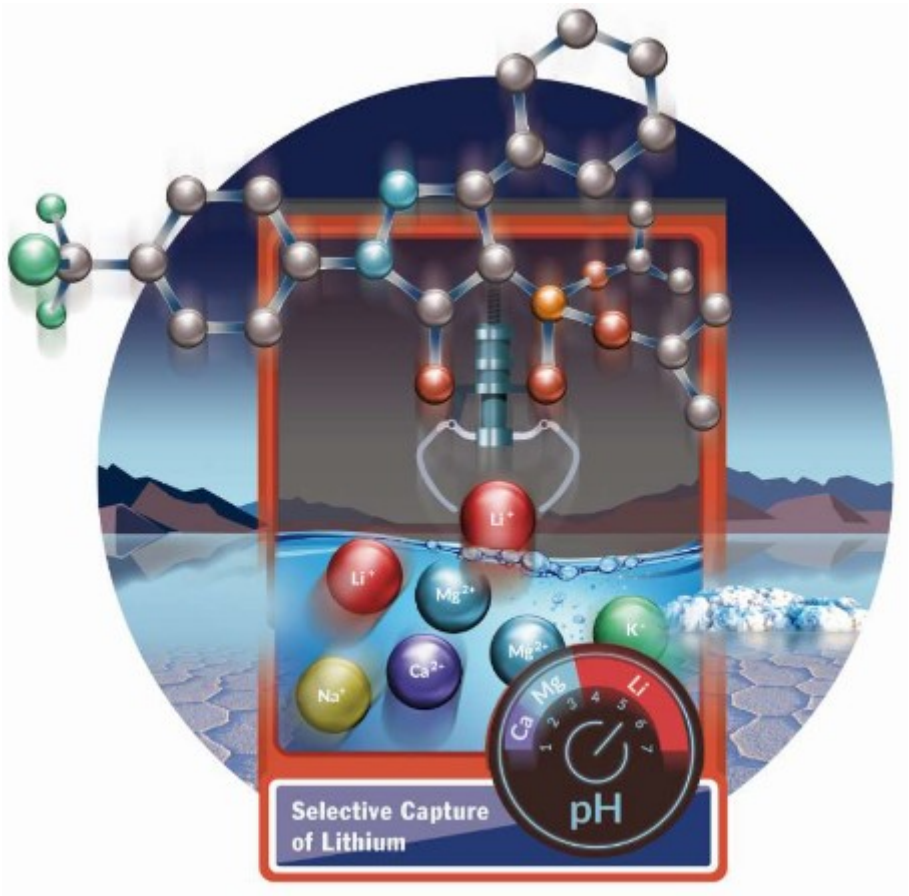
Li+
Li+
Mg2+
Mg2+
K+
Ca2-
Na+
Ca
Mg
Li
1 2 3 4 5 6 7
pH
Selective Capture
of Lithium