

Novel lithium selective 14–16 crown ether derivatives having bulky and rigid subunits: Effect of cavity size and bulky structures on alkali metal selectivity

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Novel lithium selective 14–16 membered crown-4 ethers having bulky and rigid subunits were synthesized in high yields via intermolecular cyclization of the bulky bis-epoxide intermediate with catechol under basic conditions. The structures of the synthesized intermediates and crown ethers were confirmed by NMR, FTIR, and HRMS analysis. The effect of the crown ether cavity size and different bulky subunits towards lithium selectivity was elucidated experimentally and theoretically by liquid–liquid extraction of metal perchlorates and density functional theory calculations, respectively. This work was supported by the Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT and Future Planning (2015R1A2A1A15055407) and the Ministry of Education (No. 2009–0093816).