

Design of lithium selective crown ethers with bulky and rigid subunits: Structural and selectivity studies

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A new class of lithium selective 14-crown-4 ethers having both rigid and bulky structures is reported. The rigid aromatic group provides rigidity of the 14-crown-4 ether backbone while the bulky subunit provides a blocking mechanism to prevent formation of higher ordered complexes with bigger metal ions. High yields were achieved via intermolecular cyclization of the bulky bis-epoxide 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 different bulky subunits towards lithium selectivity was elucidated by Density Functional Theory calculation and liquid-liquid extraction studies. This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Ministry of Education (No. 2009-0093816).