

Efficient Synthesis of Lithium Selective Dihydroxy-14-Crown-4 Ether with Bulky and Rigid Subunits: Experimental and Theoretical Binding Studies

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Intermolecular cyclization of bulky bis-epoxide with 1,2-dihydroxybenzene to synthesized lithium selective 14 membered crown ether 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 bigger metal ion to form a complex. The structures of the synthesized compounds were confirmed by ¹H and ¹³C NMR. The binding constants the crown ether-metal ion complex was studied using ¹H NMR titration experiments and Density Functional Theory calculation. This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Ministry of Science, ICT & Future Planning (No. 2012R1A2A1A01009683) and the Ministry of Education (No. 2009-0093816).