

Synthesis of 14–16 membered crown ether derivatives with mixed O, N, S heteroatoms:
Experimental and theoretical binding studies with platinum group metals

Torrejos Rey Eliseo[†], Jed Albarico, Grace Nisola, 민상후¹, 한정우¹, 이성풍, 정욱진
Energy and Environment Fusion Technology Center (E2FTC), Department of Energy
Science and Technology (DEST), 명지대학교; ¹Department of Chemical Engineering, 서울
시립대학교
(reytorrejos@gmail.com[†])

Efficient green synthesis of 14–15 membered crown ethers with mixed heteroatoms was synthesized via intramolecular cyclization of bis-epoxides with aromatic N or S dinucleophiles using Et₃N and metal template in H₂O. Experimental liquid-liquid extraction and DFT studies were implemented to evaluate the performance of each CEs towards Pt/Pd extraction. Among the CEs synthesized 2HDBS214C4 with $\text{\AA}_{\text{CE}}=1.58$ shows highest selectivity towards Pd ($\text{\AA}_{\text{Pd}}=1.52$) even in the presence of other platinum or precious group metals. Cavity size match relationship (CE cavity size = metal diameter) as well as changing the heteroatoms plays major role in synthesizing selective CEs for PGMs. This work was supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education (No. 2009-0093816 and 2017R1D1A1B03028102).