Supporting Materials -1

New Polyamide Cryptand for Anion Binding

Sung Ok Kang, José M. Llinares, Douglas Powell, David VanderVelde
and Kristin Bowman-James*

Department of Chemistry, University of Kansas, Lawrence, Kansas 66045
E-mail: kbowman-james@ku.edu

NMR studies:

¹H NMR spectra were recorded on a Bruker Avances 500 spectrometer at 500 MHz. Each titration was performed by 20 measurements in DMSO-*d*₆ at room temperature. Aliquots from stock solution of tetrabutylammonium salts (20 mM) were gradually added to the initial solution of ligand (2 mM). All proton signals were referred to TMS used in capillary tube. The association constants *K* were calculated by non-linear regression curve fitting program with EQNMR.¹

Figure 1. Job plots of **L** with $n\text{-Bu}_4\text{N}^+\text{Cl}^-$ (●) and $n\text{-Bu}_4\text{N}^+\text{H}_2\text{PO}_4^-$ (○) in $\text{DMSO-}d_6$ at 25 °C. Total concentration $[\text{L} + n\text{-Bu}_4\text{N}^+\text{A}^-] = 2 \text{ mM}$.

Figure 2. Partial ^1H NMR spectra of **L** in the presence of $n\text{-Bu}_4\text{N}^+\text{Cl}^-$ in $\text{DMSO-}d_6$. Numbers at the left side indicate the equivalent amounts of Cl^- added.

Figure 3. Partial ^1H NMR spectra of **L** in the presence of $n\text{-Bu}_4\text{N}^+\text{F}^-$ in $\text{DMSO-}d_6$. Numbers at the left side indicate the equivalent amounts of F^- added.