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Construction of Highly Chloride-Selective Artificial Anion Receptors

Shin-ichi Kondo

Department of Material and Biological Chemistry, Faculty of Science, Yamagata University

Summary

Recognition of chloride anion is one of the important themes in molecular recognition chemistry since chloride anion plays crucial roles in biology and environment. A cyclic bisurea derivative **2** was designed for construction of a highly chloride-selective artificial anon receptor. An important intermediate diamine **3** can be obtained from chlorobenzene in six steps in sufficient yield and **3** can be converted into diisocyanate **4** in good yield. Although the cyclization of **3** and **4** in highly diluted condition in THF was performed to give **2a**, polymeric material consisted of **3** and **4** was only obtained. A **2a** chloride adduct was successfully obtained by the reaction of **3** and **4** in the presence of tetrabutylammonium chloride as a reaction template. From the NMR analysis, a part of tetrabutylammonium in the product was substituted by other cations. These salts can be separated by solubility in chloroform. The structure of **2a**·Cl^-·tetrabutylammonium was revealed by X-ray crystallographic analysis. As expected by preliminary molecular orbital calculation, four NH of urea groups form hydrogen bonds with central chloride anion in the solid state. Two naphthyl groups of 2,2'-binaphthalene in **2a** were twisted and four 1-CH hydrogens also form weak hydrogen bonds with the chloride anion. Removal of chloride anion from **2a**·Cl^- was applied by the addition of silver nitrate, however, we can not achieve the removal of all chloride anion at this stage. Anion recognition ability of free **2a** was preliminarily elucidated by UV-vis spectroscopic titrations, chloride and bromide selectivity of **2a** can be found.