STRUCTURALLY FORCED ION BINDING AFFINITY IN A UREA-BASED MACROCYCLE

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Urea-based receptors are commonly used as potent supramolecular tools for anion recognition.[1,2] Here we report on a cyclization-driven change of complexation preferences of a urea-based receptor. Using ^{1}H NMR complexation studies, an unexpected conformation of the receptor was proposed with an electron-rich cavity formed by urea oxygens and hydrogen bond donating outer part of the macrocycle. This unique structure gives the receptor selectivity for heavier alkali metal cations, rubidium and caesium. For suitable ion pairs the obtained macrocycle functions as a ditopic receptor, causing the formation of infinite hydrogen-bound chains. Similar structures were also confirmed in the gas phase and in the solid state using high resolution mass spectrometry and X-ray crystallography, respectively.

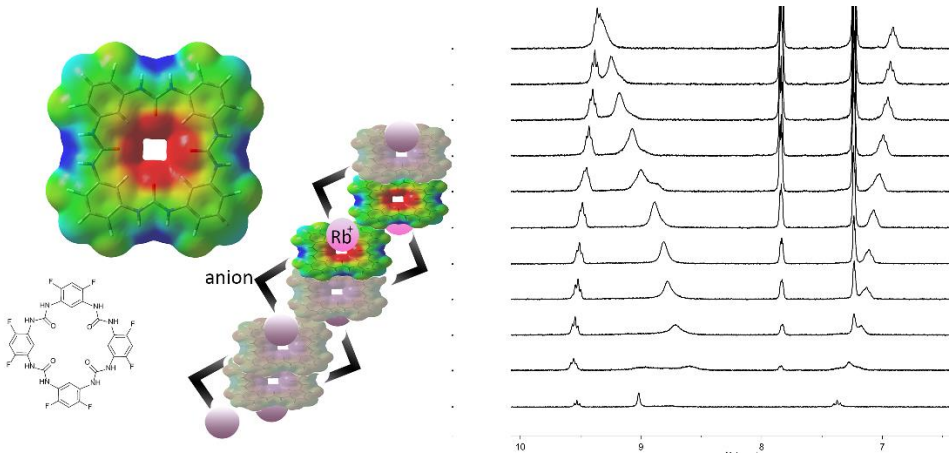

Figure 1. A urea-based ditopic receptor, left: electron density distribution in the macrocycle structure (DFT) and schematic structure of the complex with rubidium benzoate, right: ^{1}H NMR titration with rubidium benzoate.

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REFERENCES

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[2] X. Wu, P. Wang, P. Turner, W. Lewis, O. Catal, D. S. Thomas, P. A. Gale, *Chem* **2019**, *5*, 1210–122.