Computer-Aided Design and High Pressure Synthesis of Metal Ion-Sensing Molecules

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New synthetic approaches to metal ion-sensing molecules were successfully developed: (1) computer-aided design of Li^+ ion-specific "lariat ethers" and (2) high pressure synthesis of metal ion-specific "armed polyamines".

Among a variety of lariat ethers, amined armed aza-12-crown-4 derivatives formed stable and encapsulated Li^+ complexes suitable for specific recognition and transport. Since non-empirical calculations based on density functional method offered consistent results with several experimental observations, computer-aided design of a metal ion-specific lariat ether is promising.

High pressure S_NAr reaction was successfully applied to the synthesis of a new class of macrocyclic polyamines, which incorporated various heteroaromatics as potential cation binding sites on their sidearms. Since some of them exhibited high Hg^{2+} ion selectivity, this high pressure technique provides a useful method for synthesis of a new, specific receptor molecule.