A Chiral [2 + 3] Covalent Organic Cage Based on 2,2'-BINOL Units

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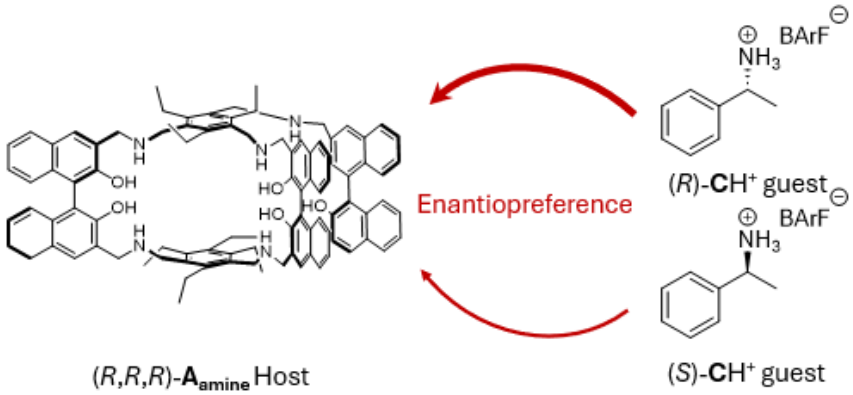
Chiral covalent organic cage is an emerging class of architectures with various applications such as gas separation, chiral separation, and catalysis.[1] Combining dynamic covalent chemistry and chiral building blocks, self-assembly of chiral cages can be achieved.[2] In this contribution, a [2+3] enantiopure covalent organic cage ($\mathbf{A}_{\mathbf{imine}}$) was synthesized through the condensation between a 3,3'-diformyl 2,2'-BINOL unit with a triamino spacer in near quantitative yields.[3] Chiral self-sorting of cage **A** was performed, and its properties were compared with a homologous cage $\mathbf{B}_{\mathbf{imine}}$ containing biphenol units. Then, the reduction of the imine bonds of cage $\mathbf{A}_{\mathbf{imine}}$ into irreversible amine bonds to increase stability permitted binding studies of cage $\mathbf{A}_{\mathbf{amine}}$ with enantiopure phenylethylammonium cations (**C**H$^+$) through UV and DOSY NMR. A higher binding constant between (*R*)-**C**H$^+$ and (*R*,*R*,*R*)-$\mathbf{A}_{\mathbf{amine}}$ compared to (*S*)-**C**H$^+$ was found which is also in agreement with molecular dynamics simulation.



Enantiopreference for the binding of (*R*,*R*,*R*)-$\mathbf{A}_{\mathbf{amine}}$ with (*R*)-**C**H$^+$ related to (*S*)-**C**H$^+$

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