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Stereoselective synthesis of cavitands and rotaxanes

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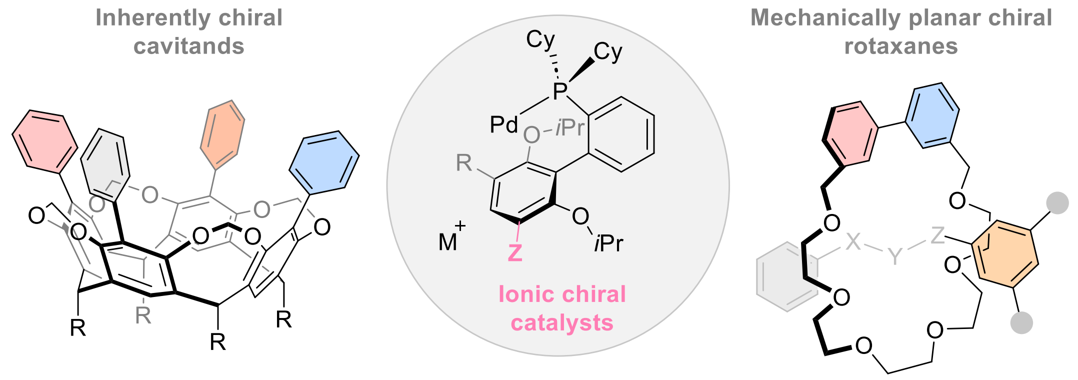
Cavitands and rotaxanes have emerged as privileged architectures in supramolecular chemistry. Nonetheless, asymmetric synthesis of inherently chiral cavitands and mechanically planar chiral rotaxanes have remained challenging. We have developed a catalytic desymmetrization strategy[1] to access enantioenriched cavitands[2] and rotaxanes[3]. Through engineering ionic chiral palladium catalysts, diverse functionalities, including aryl, alkenyl, alkynyl, and amino groups, can be installed on the rims of prochiral cavitands and on the macrocycles of prochiral rotaxanes with high stereoselectivity. Experimental and computational studies reveal synergistic electrostatic steering and electrostatic catalysis by the ionic catalyst–substrate interactions. An adaptable stepwise protocol has been established to furnish designer ABCD-type cavitands in accordance with the choreography of coupling partners. The chiral cavitand was engineered as synthetic tempate to transmit chirality to the interlocking of rotaxanes.



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