A Coordination Cage as a Crystalline Sponge

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The crystalline sponge (CS) method has emerged as an innovative X-ray technique for single-crystal diffraction analysis, eliminating the need for the traditional crystallization of analytes.[1] However, certain limitations persist, including constraints on the molecular size and polarity of analytes. In this study, we employ an M_6L_4 cage, a self-assembled molecular host with well-established host-guest chemistry,[2] as an enhanced CS to address the limitations of the original method. Large aromatic polysulfonates, or "*sticker*" anions, significantly facilitate the crystallization of the cage and circumvent the issue of static guest disorder encountered in crystallographic analysis by producing crystals in a low space group symmetry (typically, *P*-1). Benefiting from the large cavity of the cage coupled with its strong guest-binding properties, the enhanced CS allows for the analysis of a broader spectrum of analytes, including rare synthetic molecules, water-soluble molecules, and large amphiphilic molecules with a molecular weight up to ~1200.

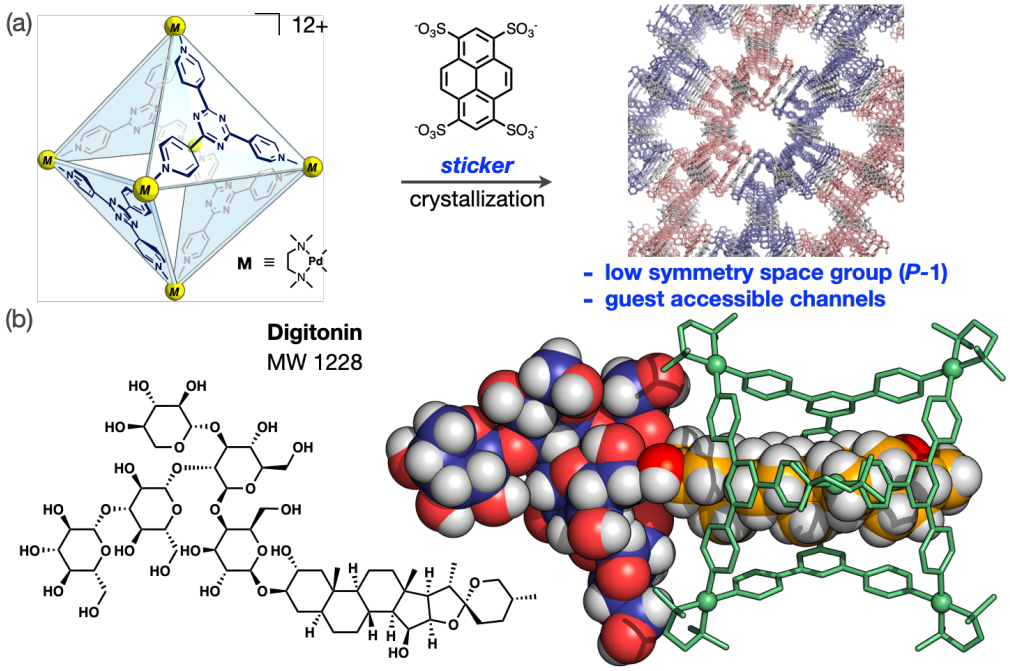

Fig.1. (a) Crystallization of an M_6L_4 cage into a potent crystalline sponge. (b) Crystal structures of guests were determined using an M_6L_4 cage as a crystalline sponge.

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