Hydrogen-Bonded Frameworks for Molecular Structure Determination

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Single-crystal diffraction is arguably the most definitive and reliable method for molecular structure determination. Yet it can be frustrated by the facts: 1) one cannot grow sufficiently large single crystals for conventional X-ray diffraction analysis, 2) many compounds form oils or amorphous phases, and 3) unstable compounds decompose under ambient conditions. Inspired by reports using "crystalline sponges," in which the structures of target molecules trapped in metal-organic frameworks have been determined by single- crystal diffraction, we report herein an complementary and straightforward approach that relies on a versatile toolkit of guanidinium organosulfonate (GS) hydrogen-bonded frameworks (HBFs) that encapsulate and wrap around target molecules to form crystalline inclusion compounds in a single step. This approach circumvents many limitations of the crystalline sponge method, relying on the peculiar properties of the GS frameworks to afford well-refined structures as well as reliable determination of absolute configuration of chiral target molecules owing to significant anomalous dispersion by sulfur atoms in the framework. The ever-expanding library of more than 100 different organosulfonates, which has produced more than 700 host-guest combination, provides a knowledge base that enables facile selection of frameworks suitable for specific target molecules based on the size and shape of the target molecules. This approach is demonstrated herein for a diverse set of host-guest combinations, illustrating the versatility and generality of using HBFs with "virtual cavities" for determination of molecular structure of target molecules.

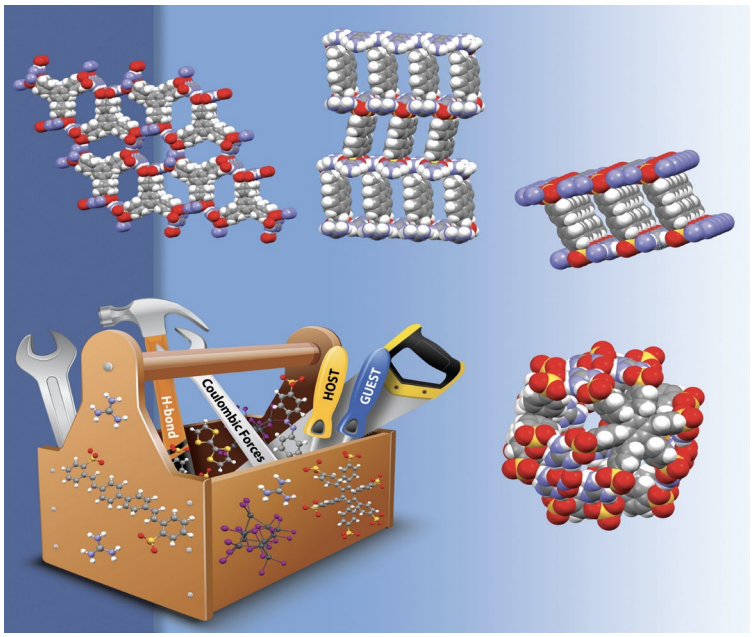

Figure 1