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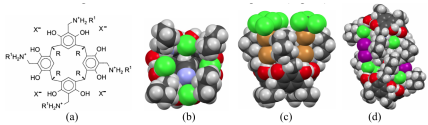

Figure 1. The chemical structure of a NARX (a), acetonitrile inclusion (b), deep cavity cavitand (c) and XB based dimeric capsule (d).

Keywords: hydrogen bonding, cavitands, resorcinaranes

MS30-O2 Organic Hydrates: Chemistry, H-Bonding & Packing

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The occurrence and understanding of hydrates (water-containing crystals) is of particular importance in the field of pharmaceutical research and industry. Hydrate formation is common for Active Pharmaceutical Ingredients (API), with one experimental polymorph screening study [1] reporting that 38% of molecules screened form hydrates and another account [2] indicating hydrates to occur for as many as 75% of drugs. This presentation will address the topic of hydration likelihood and water coordination patterns in organic hydrates, in particular with reference to pharmaceutical hydrates. We focus on the relative frequencies of hydration of specific types of molecules, re-evaluate the frequencies of occurrence and types of water coordination environment in these subsets and comment on the onward use of this information for structure evaluation and prediction.

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Keywords: hydrates, crystal engineering, hydrogen bonding