

Searching for the Best Host for Intramolecular Inclusion Among Triangular Molecules

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Investigated macrocycles were obtained through [3+3] cyclocondensation between enantiomerically pure *trans*-1,2-diaminocyclohexane and terephthalic aldehyde. Due to their triangular molecular shape and a presence of imine or amine groups, we called them accordingly as trianglimines (**1**), trianglamines (**2**) or bridged trianglamines (**3**).

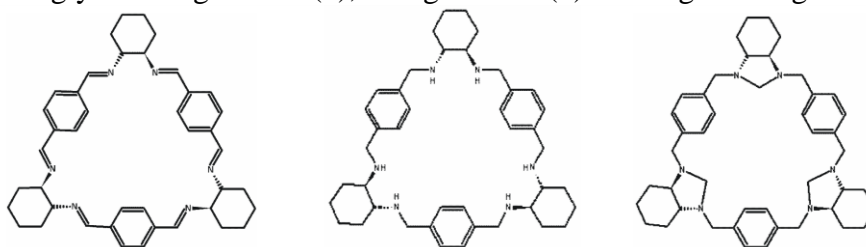


Figure 1. Examined type of host molecules: trianglimine (**1**), trianglamine (**2**) and bridged trianglamine (**3**).

In our previous work, we have investigated the ability of the three molecules to include ethyl acetate in their crystals. All three crystals displayed inclusion properties with the host molecules packed in stacks but in **1** the ethyl acetate placed itself in between the trianglimine host molecules¹ while in **2** and **3** it entered into their inner cavities. Moreover, in **2** and **3** we observed dynamic reorganization of host molecules which was implemented in two ways. In the crystals of **2** the conformationally flexible trianglamine displayed an ability to switch reversibly from an open (inclusion allowed) to a closed (inclusion prevented) state,² whereas in the crystals of **3** the bridged trianglamine crystallized with two symmetry independent host molecules and the two molecules adopted different conformations, each resembling one of the two conformational states adopted by the disordered host molecules in **2**. The above observations demonstrate that the cavity of **1** is too small to accommodate the ethyl acetate molecule, while the trianglamine host (**2**) is too flexible to allow the full control of the intramolecular inclusion. Bridged trianglamine (**3**), with rigid macrocycle and well defined inner cavity is best suited for ethyl acetate inclusion.

Therefore, our current research is focused on the investigation of intramolecular inclusion with **3** as host molecules. In this presentation we shall demonstrate the ability of this host molecule to include into its inner cavity simple alcohols such as *n*-butanol, *n*-pentanol, *n*-hexanol and *n*-heptanol, hydrocarbons *e.g.* *n*-hexane and *n*-heptane, diethyl ether and ethyl methyl ketone molecules. In majority of the investigated crystals the bridged trianglamine host molecules crystallize with two symmetry independent molecules which adopt different conformations and form channel inclusion compounds. In all crystals the channel direction is consistent with the shortest lattice direction for which the unit translation is about 5 Å or integral multiple of it. Crystallization from ethyl methyl ketone solution leads to crystals lack any inclusion and hence constitute a rare example of the porous organic material.

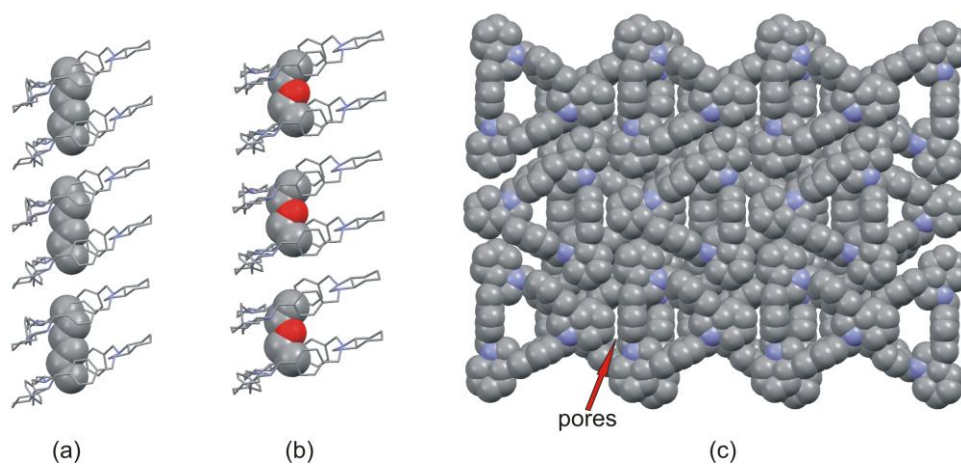


Figure 2. (a) Inclusion of *n*-hexane molecules and (b) diethyl ether molecules within the host matrices of **3**; (c) Microporosity of bridged trianglamine crystals.

Compounds for X-ray studies have been synthesized in prof. Jacek Gawroński laboratory, Department of Chemistry, Adam Mickiewicz University, Poznań, Poland

References:

1. Gawroński J., Kolbon H., Kwit M., Katrusiak A. *J. Org. Chem.*, **65** 5768 (2000).
2. Gawroński J., Gawrońska K., Grajewski J., Kwit M., Plutecka A., Rychlewska U. *Chem. Eur. J.*, **12** 807 (2006).