New Helical Host System showing True Self-inclusion

Gareth O. Lloyd^a, Leonard. J. Barbour^a, J. Alen, ^aDepartment of Chemistry, University of Stellenbosch, South Africa. ^b K.U. Leuven, Departement Chemie, Afdeling Organische Synthese, Celestijnenlaan 200F, B-3001 Leuven, Belgium. E-mail: gol@sun.ac.za

Crystal engineering of host/guest systems has been a major field of study for the last couple of decades. Even though recent studies appear to be focusing on coordination polymers, the organic host systems, such as the crown ethers, cavitands, cryptands and calixarenes, have proven to be highly successful. Due to their biological relevance, helical host systems have also been developed. The urea family and the alicyclic diol family are the most well known. The compound 2,7-dimethyl-3,5-octadiyne-2,7-diol [1] was crystallized from several solvents and single crystal X-ray diffraction analysis performed to determine whether encapsulation had occurred. The host system comprises of triple helical tubes formed via hydrogen bonding. The guest is enclathrated inside these tubes. The host shows good selectivity, as it does not encapsulate most solvents. To investigate whether the host system could be porous, crystals were grown by sublimation. The sublimed material was found to have the same host helical structure but with the host compound also inside the channels. The same self-included structure was also found when no encapsulation occurred. To our knowledge this is the first example of a host system having the same basic structure when it includes itself.

[1] Leigh D.A., Moody A.E., Pritchard R.G., *Acta Cryst. C*, 1994, C**50**, 129. Keywords: materials, supramolecular host-guest chemistry, selfinclusion