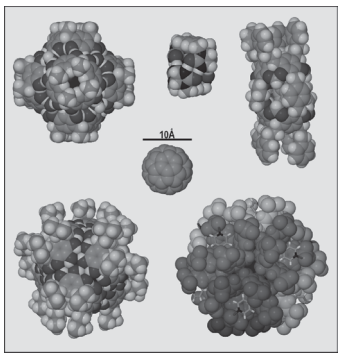
s7.m24.o5 **Enclosing Chemical Space.** Leonard J. Barbour, *Department of Chemistry, University of Stellenbosch, 7602 Matieland, South Africa, E-mail: ljb@sun.ac.za*

Keywords: Calixarenes; Encapsulation

The bottom-up assembly of elaborate structures from a relatively simple set of molecular building blocks is nowhere more beautifully exemplified than in biological systems. By exploiting the principles of supramolecular chemistry, nature has mastered the ability to form remarkably complex molecular capsules on a widely varied scale. Indeed, most of the fascinating chemistry of life-sustaining processes occurs within molecular containers such as viruses (20 to 200 nm), bacteria (1,000 to 2,000 nm) and biological cells (5,000 to 40,000 nm).



We have long been interested in the controlled assembly of large molecular capsules. Although we have derived much of our inspiration from biological systems, the formation of capsules matching the size and complexity encountered in living organisms is currently beyond the synthetic grasp of the chemist. However, we note that viral capsids consist of relatively simple geometrical arrangements of molecules (i.e. polyhedra, helices or a combination of these two morphologies). Since polyhedral arrangements of molecules are often encountered in crystals, we have based our initial approach on the study of supramolecular assemblies in the solid state. We believe that many of the principles governing the formation and stability of self-assembled containers can be unravelled by such studies. This knowledge will ultimately be applicable to the controlled assembly of molecular capsules in solution, and perhaps even in the gas phase.

s7.m25.o1 **Selectivity by Inclusion.** L R Nassimbeni, *Department of Chemistry, University of Cape Town, Rondebosch 7701, South Africa. E-mail: xrayluig@science.uct.ac.za*

Keywords: Inclusion Compounds; Selectivity; pH Control

The separation of liquids with similar boiling points by distillation is inefficient or unusable. Thus the method of selective enclathration becomes an attractive possibility. We have analysed the results of competition experiments carried out between the host Tetraphenylethanediol TPED and picoline isomers, and noted the effects of adding “neutral solvents”. The structures of the host-guest compounds were correlated to the selectivity profiles. We have also investigated the control of guest selectivity by changing the pH of the guest mixture. This was effected in the analysis of the inclusion by TPED of aniline versus benzylamine, and the host binaphthol and its inclusion of substituted quinolines. The results were related to the pK_b values of the liquid bases, and the resulting host-guest structures were elucidated.