Interactions of Supramolecular Synthons Formed by Secondary Propargylic Alcohols

Marilise A. Hyacinth, Ge Gao, Li Bin, Michal Sabat, Lin Pu, *Department of Chemistry, University of Virginia, Charlottesville, VA 22904, USA*. E-mail: mh5ua@virginia.edu

Chiral secondary propargylic alcohols are used in the enantioselective synthesis of natural products and as synthetic precursors of several optically active compounds. Secondary propargylic alcohols with aryl substituents possess three important functional groups: the hydroxyl group, the π system of the alkyne moiety, and a variety of aryl rings that can be involved in π···π stacking as well as other interactions. The combination of the three functional groups attached to one chiral carbon makes secondary propargylic alcohols well suited for applications in supramolecular chemistry and crystal engineering [1-3].

The competition between O-H…O hydrogen bonds and weaker interactions such as C-H…π and π···π stacking leads to the formation of a diverse set of synthons, including non-planar hexamers. The cooperativity between intermolecular forces is essential for the stabilization of these synthons.

[1] Desiraju G.R., *Angew. Chem. Int. Ed. Engl.,* 1995, **34**, 2311. [2] Bilton C., Howard J.A.K., Madhavi N.N.L., Nangia A., Desiraju G.R., Allen F.H., Wilson C.C. , *Acta Cryst.,* 2000, **B56**, 1071. [3] Madhavi N.N.L., Desiraju G.R., Bilton C., Howard J.A.K., Allen F.H. , *Acta Cryst.,* 2000, **C56**, 1359.

Keywords: supramolecular chemistry, crystal engineering, organic compounds