## SC12

## THERMAL ANALYSIS IN THE DESIGN OF CHIRAL RESOLUTIONS. STUDIES ON 0,0'-DIBENZOYL-(2R,3R)-TARTARIC ACID + ALCOHOL SUPRAMOLECULAR SYSTEMS

<sup>1</sup>Csaba Kassai, <sup>2</sup>Rita Illés, <sup>2</sup>György Pokol, <sup>1</sup>Dávid Kozma and <sup>1</sup>Elemér Fogassy

Department of Organic Chemical Technology, Institute of General and Analytical Chemistry, Budapest University of Technology and Economics, Budapest, P.O.B. 91, H-1521, Hungary

Dibenzoyl-(2R,3R)-tartaric acid (DBTA) is a most frequently applied resolving agent for separating racemates via diastereoisomeric salt formation on laboratory and industrial scale. It has been found recently that in several cases DBTA formed supramolecular compounds (complexes) rather than real salts with some basic racemates, and these supramolecular compounds could also be used in resolving the respective racemates (1). According to this observation we have assumed that TA and DBTA can be used for the resolution of racemate compounds without basical character too.

In the present work/thermal behaviour of DBTA, its monohydrate, and its potential supramolecular compounds with achiral alcohols, phenols and chiral alcohols were investigated with TG, DSC and EGD. The structural differences among anhydrous DBTA, its monohydrate, and the supramolecular derivatives were investigated with X-ray powder diffraction.

The thermal behaviour of DBTA supramolecular compounds with alcohols was found essentially different form that of both DBTA and its monohydrate. The DBTA: alcohol molar ratio was 1:1.01- 1:1.57 for achiral alcohols. In the case of chiral alcohols, this ratio was 1:1, in agreement with the results of a single-crystal x-ray analysis. The structure of DBTA - chiral alcohol supramolecular compounds is different from that of DBTA - achiral alcohol systems.

1. K. Nemák, M. Ács, Zs. Jászay, D. Kozma, E. Fogassy, Tetrahedron. 52 (1996) 1637.