

Abstract – Dissertation
of Glenn Damkröger on

*Silica bonded, zwitterionic
2H-Tetrazolium groups as reactive solid phases:
Synthesis, structure-property-relationship
and sorption behaviour*

Reactive solid phases based on silica gel with zwitterionic fixed ions were synthesized and characterized both structurally and sorptively. They are composed of 2,3-diphenyl-5-thio-2H-tetrazolium derivatives substituted with carboxylic-alkylic groups in *para*-position (1 to 4 methylen groups). The functional groups with a short-tethered, aliphatic spacer are distinguished by the ability of formation of inner salt structures. Conformational analysis by means of Molecular Modeling suggest that the electrostatic interactions between the two ionic compartments of the inner salts are pronounced most lowly at the 2H-tetrazolium derivatives with the carboxylic-alkyl tether located in *para* position. This structural basic requirement could lead to simultaneous sorption of cations and anions from diluted solution similar to snake-cage polymers. However, after alkaline or acidic conditions, respectively, sorption experiments towards strong inorganic electrolytes from neutral solution pointed out, that the ionic interactions do not lead to snake-cage-like behaviour, independent of the tether length of the aliphatic spacer. Consequently, the betaine-like character of the silica bonded fixed ions does not disappear due to the strong electrostatic attraction between the two ionic compartments. However, the influence of the spacer on the ionic interactions becomes apparent in sorbing $[\text{AuCl}_4]^-$ fixed to the five-membered heterocyclic ring by ion pair bonding. Atypical time-dependent loading curves indicate desorption processes and, hence, comparatively weaker interactions taking effect additionally. As a result, adsorptive dipole-induced-dipole interactions as well as the formation of ionic associates and mechanisms of solvation and replacement could be a factor.

The investigations of non-ionic interactions of the solid phases towards neutral organic analyte molecules from dilute solution demonstrated that the modified silica phases are extreme polar normal phases also being provided with hydrophobic interactions. These amphiphilic properties are influenced by the tether length of the aliphatic spacer presenting the chance of systematically controlling the surface polarity of the solid phases.