

International Conference on

Applied Crystallography

October 17-19, 2016 Houston, USA



Gerd Kaupp

University of Oldenburg, Germany

Crystal structure and organic solid state reactions

Crystal structures of organic solid-state reactions are decisive for their occurrence and selectivity. While, Schmidt's topochemistry concentrates on a distance limit between reacting centers by denying molecular migrations within the crystal, too many positive and negative failures pose unsurmountable problems for predictions. Conversely, AFM, SNOM, GID, and nano-scratching indicate anisotropic molecular migrations, enforced by the internal pressure upon chemical change by reaction that requires release. This holds for intra- and inter-crystalline and for gas-solid reactions also with formerly "too large" distances, explains non-reactivities at very small distances, and inter-crystalline reactions. Crystallographic possibilities are required for molecular migrations within slip-planes and channels, or to sufficiently widen the crystallographic voids. Such migrations are anisotropic and they are face-specific. Slip-planes or channels end on the reactive crystal faces, not on the unreactive ones. For intra-crystalline reactions, molecules move out and for inter-crystalline ones reactants also move in. Solid-state reactions profits from the bargain of favorable crystallinity with respect to the same melt reactions (the latter require up to about 100K higher temperature and are less selective). This opposes undue beliefs that solid-state reactions needs to be molten, or claims that these should require "help by some solvent". Such widely proposed beliefs restrict to reactions that proceed around room temperature as liquid-state reactions, mostly loosing completeness and/or specificity. In the case of non-reactive polymorphs one may try to generate and use different modifications. The pseudo-problems of topochemistry are easily removed by applying the full structural content. New applications for molecular and polymer (including large-scale) chemistry ensue.

Biography

Gerd Kaupp has completed his PhD from Würzburg University and Post-doctoral studies from Iowa State, Lausanne and Freiburg University. He was a Full Professor till 2005 in Oldenburg, Germany, and now he privately continues his research on Solid State Reactions, AFM on rough surfaces (since 1988), the as yet better resolving sub-diffraction limit microscopy also for non-fluorescing materials, even rough ones, of all types (resolution <10 nm, since 1995), and nano-indentations (since 2000). He has published more than 300 papers in renowned journals and has been serving as an Editorial Board Member of several scientific journals.

gerd.kaupp@uni-oldenburg.de

Notes: