

# Review, New Insights and Selected Examples of Desolvation Investigations

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Some years ago, we have published a unified model for the dehydration of molecular crystals [1]. At this time, we were already convinced that this model was not an end product, and should be further discussed, criticized, extended and improved.

Since, we have investigated the thermal behavior and the physical characteristics of various compounds able to form hydrates and solvates. This extension to desolvation processes has included the study of solvent exchanges which can be either controlled by the vapor pressure of a solvent around particles [2] or conducted in far-from-equilibrium conditions [3], inducing then the kinetically-controlled formation of unexpected crystal forms with the shape of whiskers. The peritectic decomposition of a new  $\alpha$ -lactose solvate has also been observed, due to the low vapor pressure of the used solvent [4].

In the literature, recent papers have highlighted the increase of the proportion of organic solvates among molecular crystals [5]. This increase provides the opportunity to get deeper insights into the processes of solid-solid transformations involving solvent molecules. In the case of hydrates, several models or classifications have been published as attempts to rationalize the dehydration behaviors. The classifications proposed by Morris [6] and Mimura [7] are based on structural data and take into account the location and the interactions between solvent molecules in the crystal packings. These data can, in some cases, explain the thermal behaviors, for instance when the departure of water molecules requires the almost complete disruption of the packing. By contrast, the model proposed by Galwey [8] is mainly derived from kinetic studies devoted to inorganic hydrates. A major interest of this model is that the role of reaction interfaces is emphasized, allowing to account for various observations such as the progressive formation of new amorphous or crystalline materials, as well as the possible appearance of waterproof layers.

Therefore, the present contribution proposes an overview of the models and classifications already published, with the aim to highlight some of their benefits and limitations. A few illustrative examples are used to show that further progress in the understanding of desolvation mechanisms should take into account physical and environmental parameters such as the size of the studied particles and the atmosphere or surrounding medium in which the sample is placed. Furthermore, we suggest that an improved knowledge of possibly decisive steps during desolvations requires a detailed characterization of initial and final situations, but also an analysis of intermediate states which can determine the evolution of the system during the desolvation process.

## References

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