

## **Packing polymorphs and high Z' structures obtained by different crystallization conditions**

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At present relative orientation of molecules in crystals and formation of strong 1D and 2D intermolecular associates as well as ways of modification of molecular packing by crystallization conditions attract significant interest. Such interest is caused by possibility of variations of crystalline properties based on type of molecular packing. In this project a large series of planar heteroaromatic molecules was considered to evaluate how crystallization conditions might modify molecular arrangements in crystals.

It was found that in dependence on crystallization conditions (crystallization from solution or from gas phase as well as presence of additives) produced several packing polymorphs for phenazine derivatives with H and Halogen substituents. It was also indicated that for these materials quite common is presence of several (up to six) symmetrically independent molecules in one crystal.

Comparison of the calculated lattice energies for polymorphs revealed insignificant energy differences between the polymorphs, thus explaining the existence of the large number of polymorphs in this series of materials.