MS24-P1 **Polymorphic behaviour of 5-chloro-3-phenyl-2(1*H*)-pyrazinone** Liliana Dobrzańska,[ab] Jo Alen,[a] W. M. De Borggraeve[a] [a]*Department of Chemistry, KU Leuven, Celestijnenlaan 200F bus 2404, B-3001 Heverlee, Belgium,* [b]*Department of Chemistry and Polymer Science, University of Stellenbosch, Private Bag X1, Matieland 7602, Stellenbosch, South Africa*
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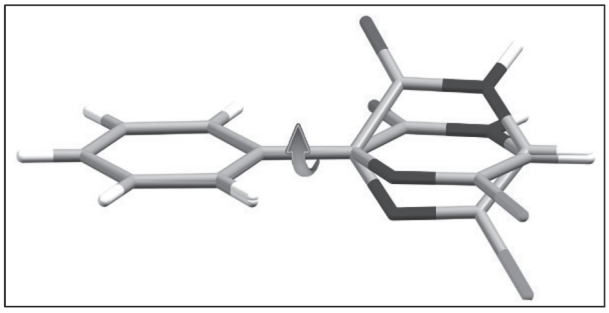
2(1*H*)-Pyrazinones are attractive scaffolds, both as templates and as starting materials for heterocycles' construction. [1] Some of the fomer show very promising activity as *í*-opioid receptor agonists, and NNRTI's (non-nucleoside reverse transcriptase inhibitors). Besides this intrinsic value, they can also be transformed into a useful tool for the synthesis of 'modified' peptides. [2]

In continuation of our studies on 2(1*H*)-pyrazinones, [3] solid-state characterisation allowed to separate two conformational polymorphs of 5-chloro-3-phenyl-2(1*H*)-pyrazinone, the crystal growth of which was influenced by temperature. Form **I** crystallises from a methanol solution at room temperature in the monoclinic space group *P*21/*c*, whereas form **II** crystallises at low temperature in the centrosymmetric triclinic space group with two independent molecules in the asymmetric unit. Single-crystal XRD revealed that two aromatic rings are coplanar in **I** but show a twist around the C-C bond in **II**. The results of PXRD studies as well as an analysis of the intermolecular interactions in the packing will be presented.



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Keywords: pyrazinones; polymorphs; intermolecular interactions

MS24-P2 **Hydrogen/deuterium-exchange on small organic molecules and its influence on the molecular aggregation.** *Anna Kupka, Vera Vasylyeva, Klaus Merz* , Department of Inorganic Chemistry I, Ruhr-University Bochum, 44801 Bochum, Universitätsstrasee 150, Germany*
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How well do we currently understand the aggregation of small molecules in the solid state? Most of intermolecular interactions are not very strong and their formation is related to and affected by small changes in the molecular structure and the crystallisation conditions. Continuing our investigations on aggregation of substituted aromatic molecules in the solid state, we studied the influence and boundaries of weak directing substituents like deuterium on the aggregation of small molecules. Hydrogen/deuterium (H/D)-exchange, the smallest possible modification of a molecule, is generally seen as a non dominating parameter in the formation of crystal structures of chemical compounds. On the other hand, we can show that the aggregation of molecules in the solid state of polymorphic N-heterocycle systems like pyridine-N-oxide or acridine or even benzidine can be very sensitive on small changes of the isotopic substitution pattern of the well selected molecules. One amazing example is pyridine. An isotopic substitution leads to the formation of a new polymorph. Re-crystallisation from pentane allows the formation of a new stable polmorph of pentadeuteropyridine [1]. Our own recent investigations of partially deutero-substituted pyridine-N-oxides yield two different polymorphs for a partial deuterated compound. Both the low-temperature and the high-temperature phases are stable and reversible [2,3]

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Keywords: deuterium effect; structural polymorphism; small organic molecules