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Preferred isomerism of hydroxy-N,N'-diarylformamidine derivatives in the solid-state

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Introduction
The flexibility of diarylformamidine ligands to coordinate either as monodentate or as chelating ligands render their respective complexes very promising for application in catalysis [1]. N-hydroxy-N,N'-diarylformamidine complexes have been reported by our research group to be significant initiators in ring opening polymerization [2]. In this work, we explore the synthesis and characterization of hydroxy-N,N'-diarylformamidine derivatives with particular interest in their preferred isomerism in the solid-state.

Results
Symmetrical and Unsymmetrical N-hydroxyformamidines were synthesized and characterized using various spectroscopic techniques. The crystals of the compounds obtained underwent X-ray diffraction analysis, revealing that symmetrical formamidines can adopt both zwitterionic and neutral hydroxy forms, whereas unsymmetrical compounds exclusively adopt the zwitterionic form in solid state. The zwitterions exhibit Zanti isomerism, while the neutral hydroxy forms exhibit Eanti isomerism. Symmetrical and unsymmetrical compounds with smaller substituents tend to form dimeric molecular units, described by an R_2ˆ2 (10) graph set descriptor. In contrast, unsymmetrical compounds with bulkier substituents form chain-like structures. Classical hydrogen bonds (N–H…O, N—H…N, N—H…O, and O–H…N) stabilize the crystal packing in dimeric units, while C–H…O interactions promote packing in chain-forming molecules. Pairwise interaction energy calculations reveal that electrostatic energy (Eele) predominates in the stability of the dimeric pairs, whereas dispersion energy (Edis) is more dominates in chain-like structures.

References
[1] Akpan ED, Ojwach SO, Omondi B, Nyamori VO., New J. Chem. **40** (2016) 3499-3510.
[2] Munzeiwa WA, Omondi B, Nyamori VO, Polyhedron. **138** (2017) 295-305.

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