MS29-1-3 Polymorphism in a series of dipodal N-donor ligands containing a biphenyl core
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Abstract
Polymorphism[1] is the ability of a substance to form various crystalline phases that differ for example by their molecular arrangement (packing polymorphism)[2] or by the molecular conformation they adopt (conformational polymorphism)[3]. It is known that varying the conditions (change of solvent, level of supersaturation, temperature, pressure) during the crystallization process is the main factor responsible for this phenomenon to occur, leading to the formation of products displaying different physical properties, including thermodynamic, spectroscopic, kinetic and mechanical characteristics[4]. Unfortunately, polymorphism is far from being clearly understood. Computational studies such as crystal structure predictions (CSP), which are under continuous development to complement the experimental screening of solid forms, help to identify the most likely formed polymorphic phases and to understand the crystallization behaviour at the molecular level[5].
Herein, we would like to present the polymorphic behaviour of a series of flexible dipodal N-donor ligands containing a biphenyl core, namely 4,4′-bis(pyridin-4-ylmethyl)-1,1′-biphenyl **(1)**, 4,4′-bis(1H-imidazol-1-ylmethyl)-1,1′-biphenyl **(2)** and 2,2′-bis(1H-imidazol-1-ylmethyl)-1,1′-biphenyl **(3)**. Crystals of these heterocyclic ligands were grown from a range of solvents such as THF, MeOH, DCM, EtOH, acetonitrile, and acetone. Two different forms for each of the ligands were isolated and their crystal structures were determined by SCXRD analysis. These were further profiled by various techniques such as TGA/DTA, powder XRD, FT-IR and computational methods, with the latter providing better understanding of the interplay of the intermolecular interactions.

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