Supporting Information

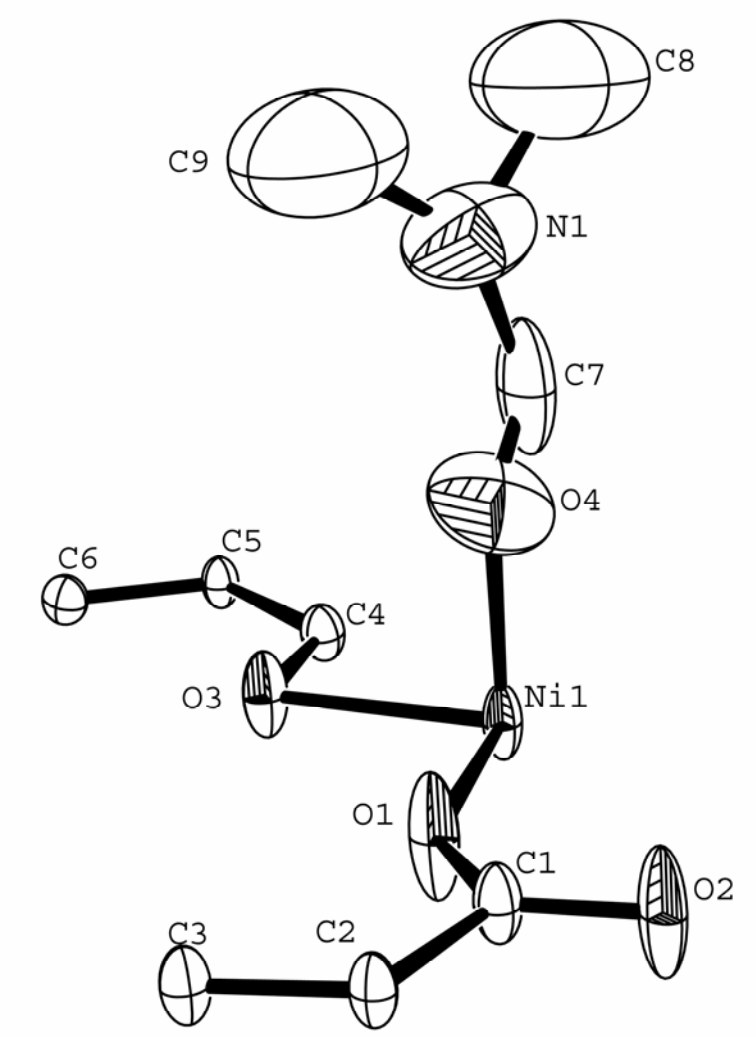

Fig. S1 ORTEP view of the compound **1** with thermal ellipsoids at 30% level. Disordered part has not been shown for clarity.

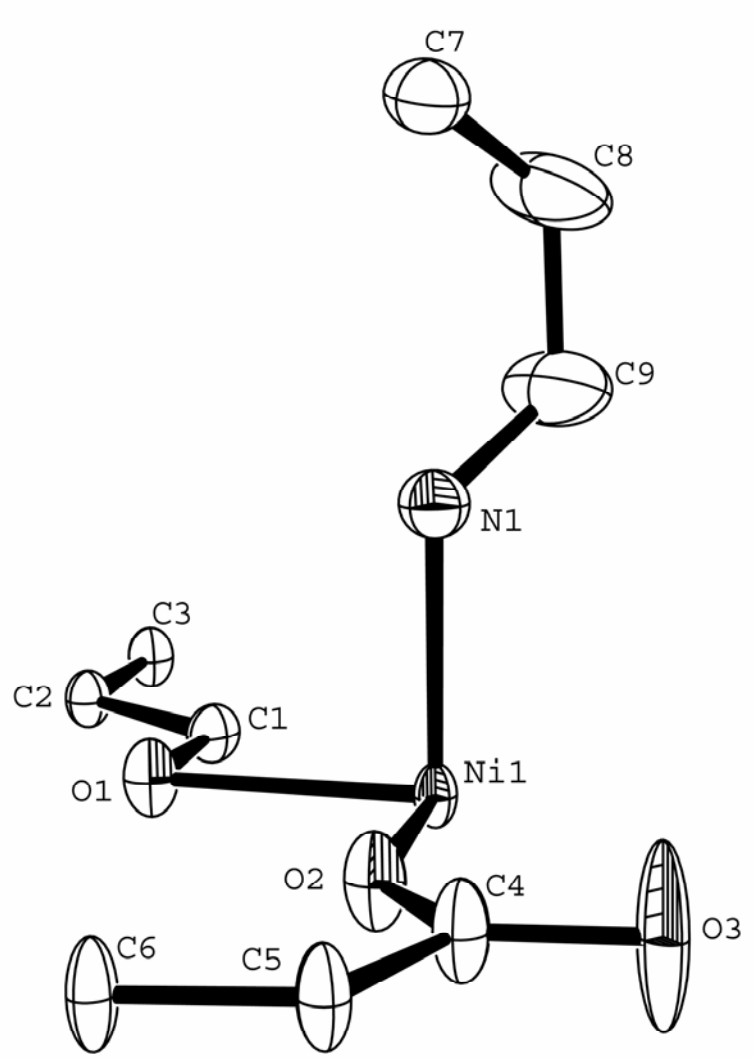

Fig. S2 ORTEP view of the compound **2** with thermal ellipsoids at 30% level. Disordered part has not been shown for clarity.

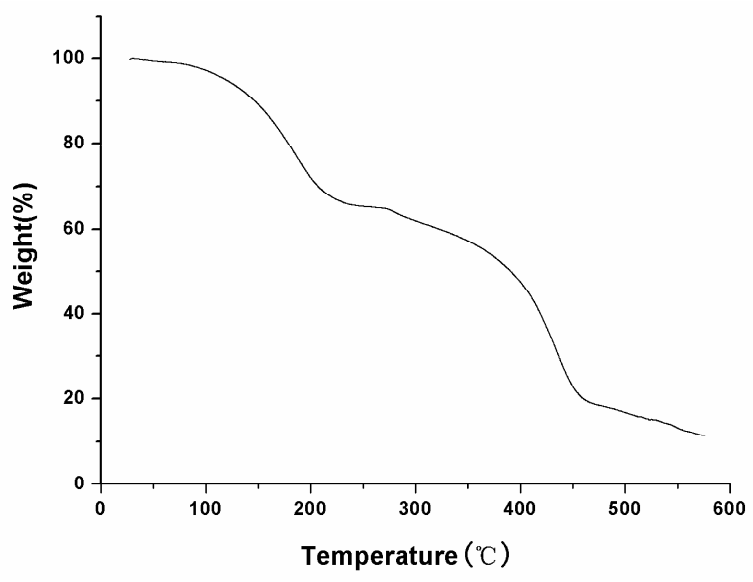

Fig. S3 TG curve of as-synthesized **2**. Heating rate: 10 deg sec^{-1}, N_2 atmosphere temperatures. The TGA curve shows release of guest DMF molecules between that 25 and 235 °C leading to a weight loss of 34.11%, which suggests a pore filling of 3 DMF molecules per Ni centre. Above 235 °C, the sample shows no further weight loss up to 272 °C at which temperature the compound decomposed.

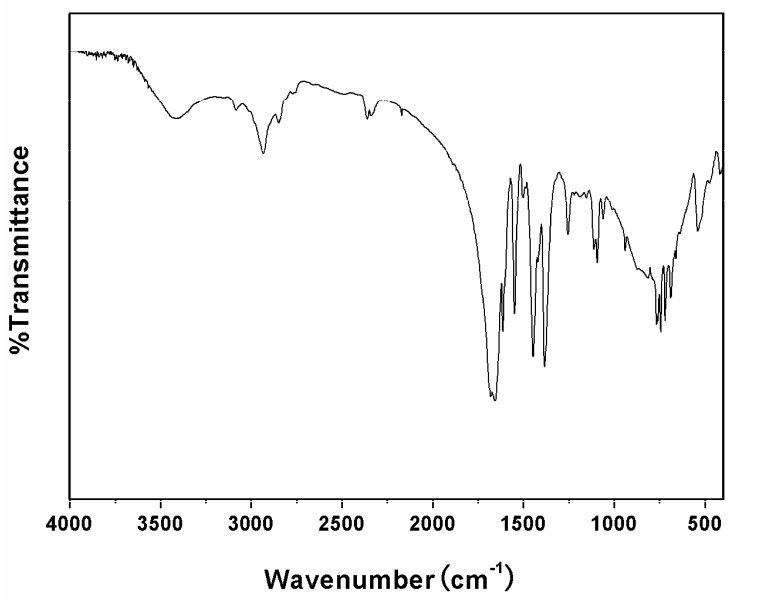

Fig. S4 FT-IR spectrum of as-synthesized sample **1**.

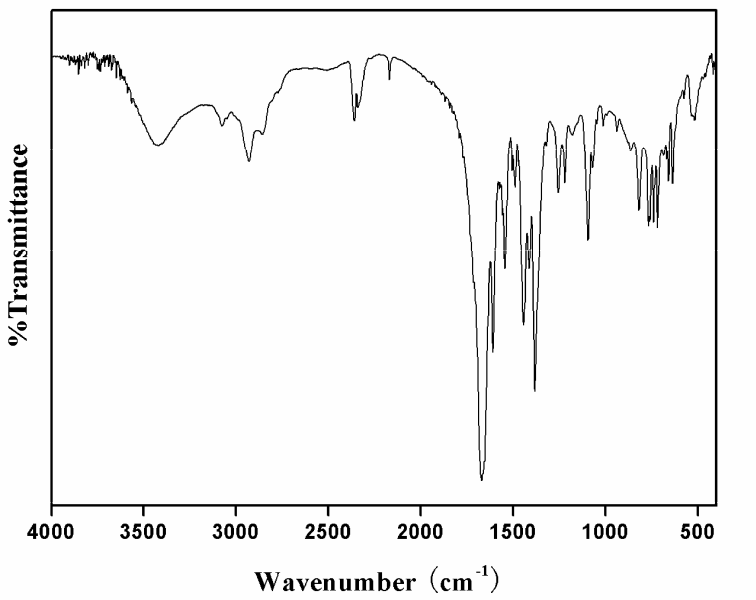

Fig. S5 FT-IR spectrum of as-synthesized sample **2**.

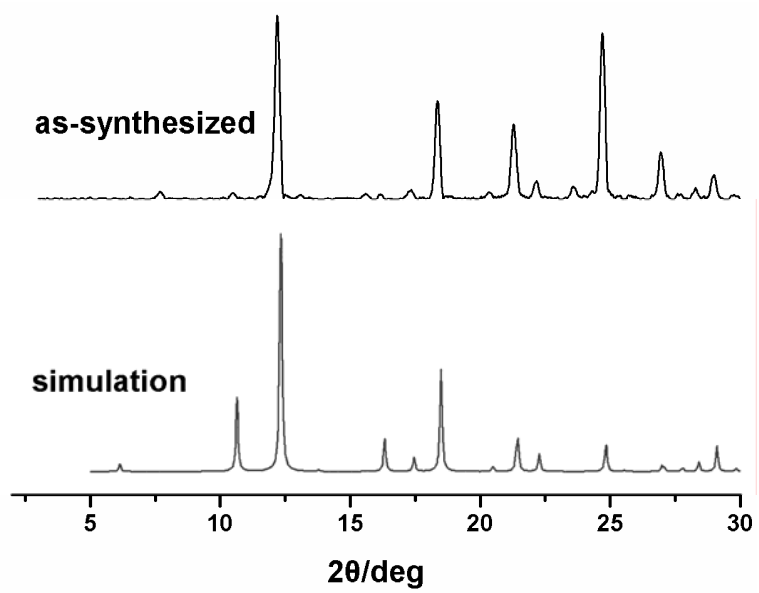

Fig. S6 XRPD patterns of the as-synthesized samples **1** and the simulation based on the single-crystal data of **1**.

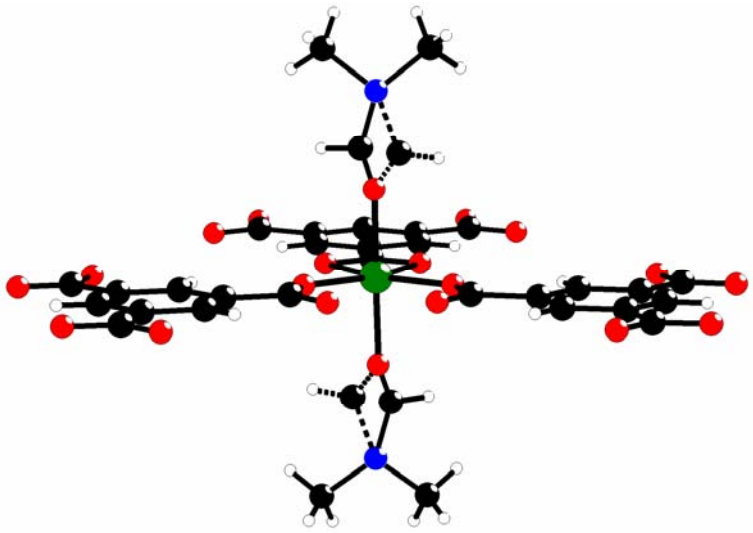

Fig. S7 The DMF molecules disorder at two positions in **1**.

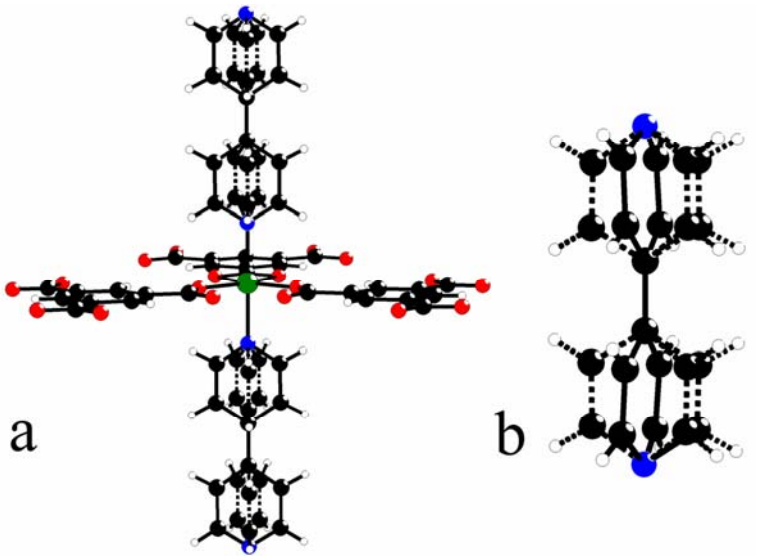

Fig. S8 4,4'-bipy ligands disorder at three positions along the threefold axis in compound **2**.