

Supplementary Information

for

Screening polymorphism in Ni(II) metal-organic framework: Experimental observations, Hirshfeld surface analyses and DFT studies

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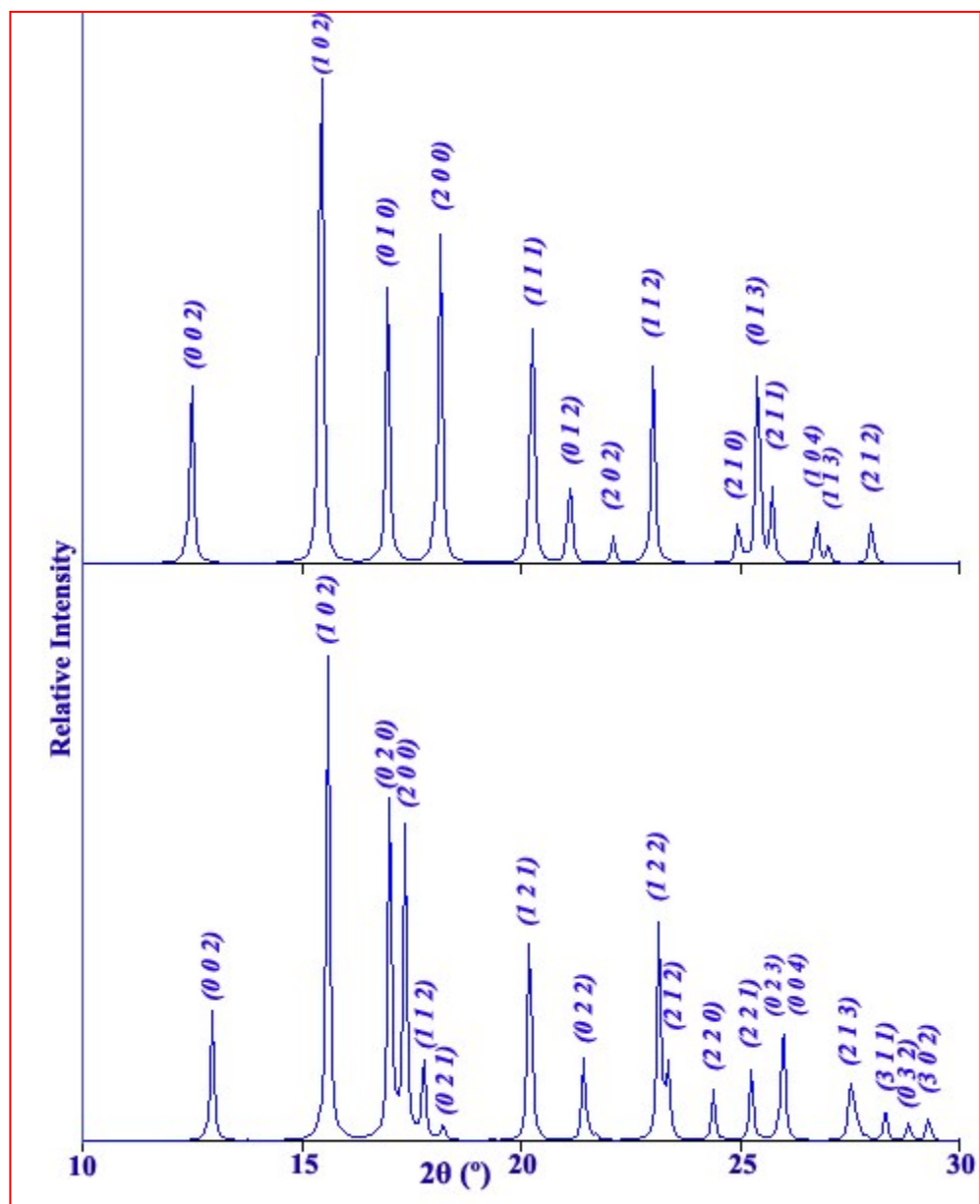


Fig. S1 Calculated powder diffraction of Form-I (top) and form-II (bottom).

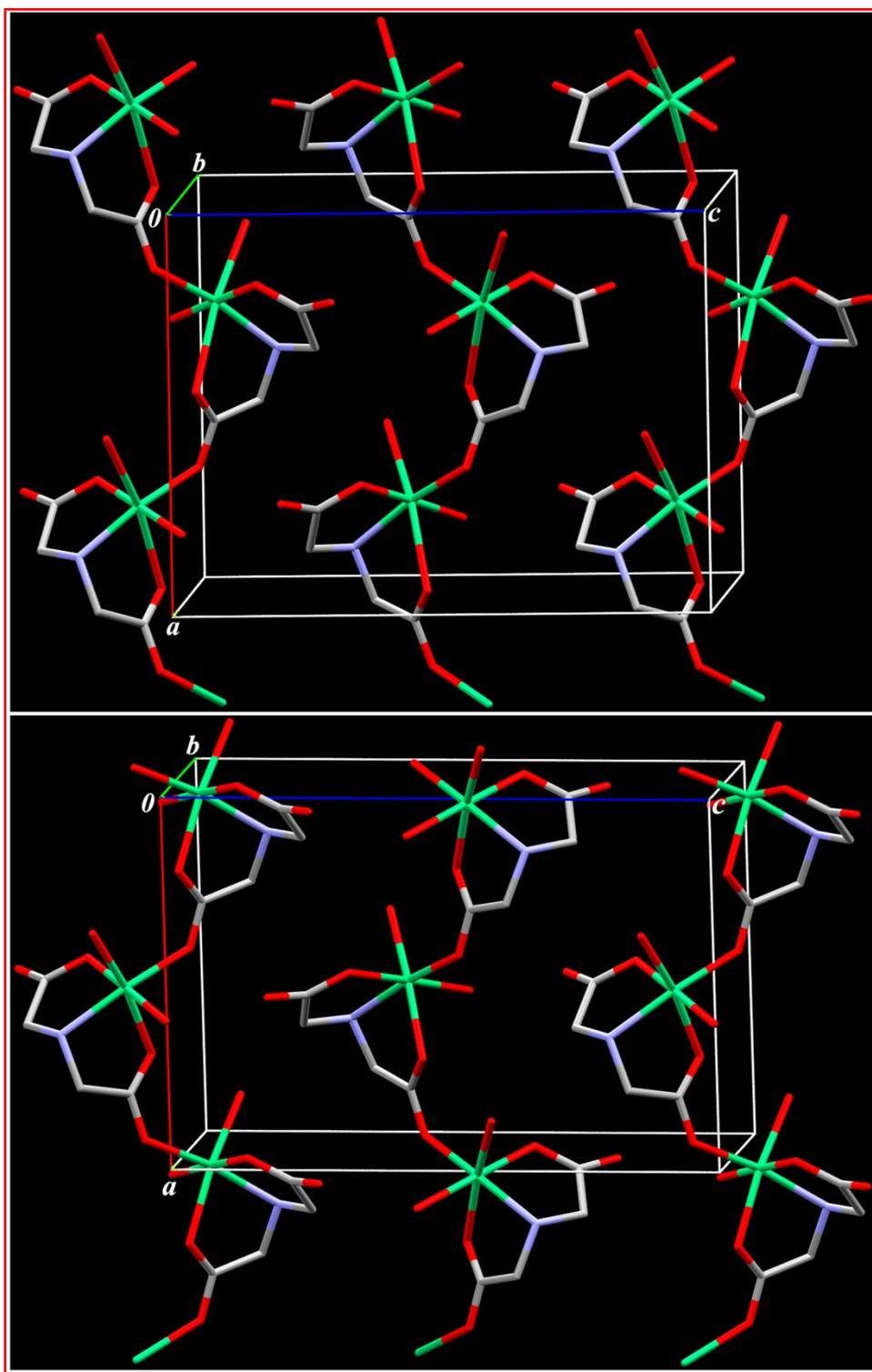


Fig. S2 Propagation of parallel polymeric chains along $(1\ 0\ 0)$ direction for Form-II (top) and form-I (bottom).

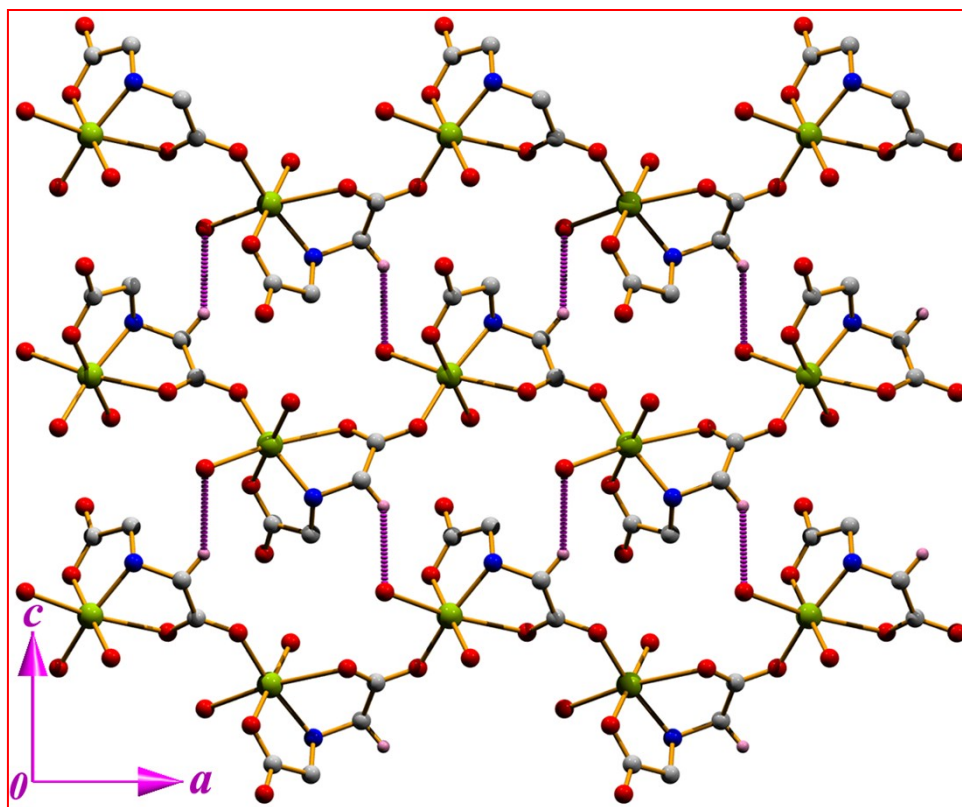


Fig. S3 Perspective view of supramolecular layered assembly generated through weak C–H...O hydrogen bonding interaction in form-**II**.

Table S1. Bond lengths and bond angles for the two polymorph I and II (Å, °).

Bond lengths and angles	Form-II (L.T)	Form-II (R.T)	Form-I (WADNUL)
Ni(1) – O(1)	2.493(2)	2.492(3)	2.123(4)
Ni(1) – O(2)	1.961(2)	1.958(9)	2.011(4)
Ni(1) – O(3)	1.945(2)	1.938(9)	2.027(4)
Ni(1) – O(1W)	2.408(3)	2.410(4)	2.087(4)
Ni(1) – O(2W)	1.978(2)	2.002(7)	2.112(4)
Ni(1) – N(1)	2.014(2)	1.994(8)	2.055(5)
O(1) – Ni(1) – O(2)	93.7(1)	93.78(12)	90.5(2)
O(1) – Ni(1) – O(3)	91.5(1)	91.76(14)	92.8(2)
O(1) – Ni(1) – O(1W)	167.9(1)	167.95(11)	169.0(2)
O(1) – Ni(1) – O(2W)	86.8(1)	86.36(12)	85.7(2)
O(1) – Ni(1) – N(1)	73.1(1)	72.56(11)	79.1(2)
O(2) – Ni(1) – O(3)	88.0(1)	87.73(18)	88.2(2)
O(2) – Ni(1) – N(1)	165.1(1)	164.91(18)	166.4(2)
O(2) – Ni(1) – O(1W)	97.5(1)	97.33(14)	99.2(2)
O(2) – Ni(1) – O(2W)	91.3(1)	90.17(16)	91.7(2)
O(3) – Ni(1) – O(1W)	93.6(1)	93.35(15)	92.7(2)
O(3) – Ni(1) – N(1)	85.5(1)	86.36(21)	83.6(2)
O(3) – Ni(1) – O(2W)	178.1(1)	177.08(18)	178.5(2)
O(1W) – Ni(1) – O(2W)	88.3(1)	88.93(13)	88.8(2)
O(1W) – Ni(1) – N(1)	96.4(1)	96.87(13)	92.0(2)
O(2W) – Ni(1) – N(1)	94.8(1)	95.18(19)	96.2(2)