Supporting Information for Crystal Growth & Design

Coordination Frameworks Containing Magnetic Single Chain of Imidazoledicarboxylate-Bridged Cobalt(II)/Nickel(II): Syntheses, Structures, and Magnetic Properties

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Table S1. Selected bond lengths (Å) and angles (°) for **1**−**5**.

1			
Co1−O5A	2.118(4)	Co1−O(5)	2.118(4)
Co1−N1A	2.120(4)	Co1−N1	2.120(4)
Co1−O1	2.129(3)	Co1−O1A	2.129(3)
Co2−O(6)	2.062(4)	Co2−O6B	2.062(4)
Co2−N2	2.147(4)	Co2−N2B	2.147(4)
Co2−O4B	2.149(4)	Co2−O4	2.149(4)
O5A−Co1−O5	180.0	O5A−Co1−N1A	92.3(2)
O5−Co1−N1A	87.7(2)	O5A−Co1−N1	87.7(2)
O5−Co1−N1	92.3(2)	N1A−Co1−N1	180.0
O5A−Co1−O1	88.8(2)	O5−Co1−O1	91.2(2)
N1A−Co1−O1	100.7(1)	N1−Co1−O1	79.3(1)
O5A−Co1−O1A	91.2(2)	O5−Co1−O1A	88.8(2)

N1A−Co1−O1A	79.3(1)	N1−Co1−O1A	100.7(1)
O1−Co1−O1A	180.0	O6−Co2−O6B	180.0(1)
O6−Co2−N2	91.0(2)	O6B−Co2−N2	89.0(2)
O6−Co2−N2B	89.0(2)	O6B−Co2−N2B	91.0(2)
N2−Co2−N2B	180.0(1)	O6−Co2−O4B	89.6(2)
O6B−Co2−O4B	90.5(2)	N2−Co2−O4B	101.3(1)
N2B−Co2−O4B	78.7(1)	O6−Co2−O4	90.5(2)
O6B−Co2−O4	89.6(2)	N2−Co2−O4	78.7(1)
N2B−Co2−O4	101.3(1)	O4B−Co2−O4	180.0(2)
		2	
Ni1−N1A	2.066(3)	Ni1−N1	2.066(3)
Ni1−O(1)	2.102(3)	Ni1−O1A	2.102(3)
Ni1−O5A	2.109(3)	Ni1−O5	2.109(3)
Ni2−O6	2.071(3)	Ni2−O6B	2.071(3)
Ni2−O4B	2.092(3)	Ni2−O4	2.092(3)
Ni2−N2B	2.104(3)	Ni2−N2	2.104(3)
N1A−Ni1−N1	180.0	N1A−Ni1−O1	99.3(1)
N1−Ni1−O1	80.7(1)	N1A−Ni1−O1A	80.7(1)
N1−Ni1−O1A	99.3(1)	O1−Ni1−O1A	180.0
N1A−Ni1−O5A	91.8(1)	N1−Ni1−O5A	88.2(1)
O1−Ni1−O5A	87.9(1)	O1A−Ni1−O5A	92.1(1)
N1A−Ni1−O5	88.2(1)	N1−Ni1−O5	91.8(1)
O1−Ni1−O5	92.1(1)	O1A−Ni1−O5	87.9(1)
O5A−Ni1−O5	180.0(1)	O6−Ni2−O6B	180.0(2)
O6−Ni2−O4B	89.5(1)	O6B−Ni2−O4B	90.5(1)
O6−Ni2−O4	90.5(1)	O6B−Ni2−O4	89.5(1)
O4B−Ni2−O4	180.0(1)	O6−Ni2−N2B	91.7(1)
O6B−Ni2−N2B	88.3(1)	O4B−Ni2−N2B	80.7(1)
O4−Ni2−N2B	99.3(1)	O6−Ni2−N2	88.3(1)

O6B−Ni2−N2	91.7(1)	O4B−Ni2−N2	99.3(1)
O4−Ni2−N2	80.7(1)	N2B−Ni2−N2	180.0(1)
		3	
Co1−N1A	2.126(4)	Co1−N1	2.126(4)
Co1−O1A	2.143(4)	Co(1)-O(1)	2.143(4)
Co1−N4B	2.155(6)	Co1−N3	2.158(7)
N1A−Co1−N1	179.7(2)	N1A−Co1−O1A	80.3(1)
N1−Co1−O1A	99.7(1)	N1A−Co1−O1	99.7(1)
N1−Co1−O1	80.3(1)	O1A−Co1−O1	176.6(2)
N1A−Co1−N4B	89.8(1)	N1−Co1−N4B	89.8(1)
O1A−Co1−N4B	91.7(1)	O1−Co1−N4B	91.7(1)
N1A−Co1−N3	90.3(1)	N1−Co1−N3	90.2(1)
O1A−Co1−N3	88.3(1)	O1−Co1−N3	88.32(10)
N4B−Co1−N3	180.0(1)		
		4	
Co1−N7A	2.088(7)	Co1−N4	2.120(7)
Co1−N1	2.129(6)	Co1−O4B	2.137(5)
Co1−N2B	2.142(6)	Co1−O1	2.170(6)
N7A−Co1−N4	92.1(3)	N7A−Co1−N1	96.4(3)
N4−Co1−N1	163.9(3)	N7A−Co1−O4B	90.5(2)
N4−Co1−O4B	98.1(3)	N7A−Co1−O1	92.4(2)
N1−Co1−O4B	95.5(2)	N7A−Co1−N2B	169.0(3)
N4−Co1−N2B	86.9(3)	N1−Co1−N2B	87.4(2)
O4B−Co1−N2B	78.7(2)	N4−Co1−O1	87.4(3)
N1−Co1−O1	78.6(2)	O4B−Co1−O1	173.7(2)
N2B−Co1−O1	98.5(2)		
		5	
Ni1−N4	2.055(8)	Ni1−N7A	2.080(7)
Ni1−N2B	2.094(7)	Ni1−N1	2.108(9)

Ni1−O1	2.11(1)	Ni1−O4B	2.12(1)
N4−Ni1−N7A	91.8(4)	N4−Ni1−N2B	95.3(3)
N7A−Ni1−N2B	166.5(2)	N4−Ni1−N1	169.5(2)
N7A−Ni1−N1	87.2(4)	N2B−Ni1−N1	87.9(4)
N4−Ni1−O1	89.6(4)	N7A−Ni1−O1	96.5(3)
N2B−Ni1−O1	95.0(3)	N1−Ni1−O1	80.1(3)
N4−Ni1−O4B	93.3(4)	N7A−Ni1−O4B	87.7(3)
N2B−Ni1−O4B	80.5(3)	N1−Ni1−O4B	97.1(3)
O1−Ni1−O4B	174.9(1)		

Symmetry codes: A = 2 − *x*, − *y*, 1 − *z*; B = 1 − *x*, 1 − *y*, 1 − *z* for **1**. A = − *x*, 2 − *y*, 1 − *z*; B = 1 − *x*, 1 − *y*, 1 − *z* for **2**. A = *x*, 1/2 − *y*, 1 − *z*; B = −1 + *x*, *y*, *z* for **3**. A = 1 − *x*, 1 − *y*, 1 − *z*; B = 3/2 − *x*, − 1/2 + *y*, 3/2 − *z* for **4**. A = − *x*, 1 − *y*, − *z*; B = 1/2 − *x*, 1/2 + *y*, 1/2 − *z*; C = 1 − *x*, − *y*, − *z* for **5**.

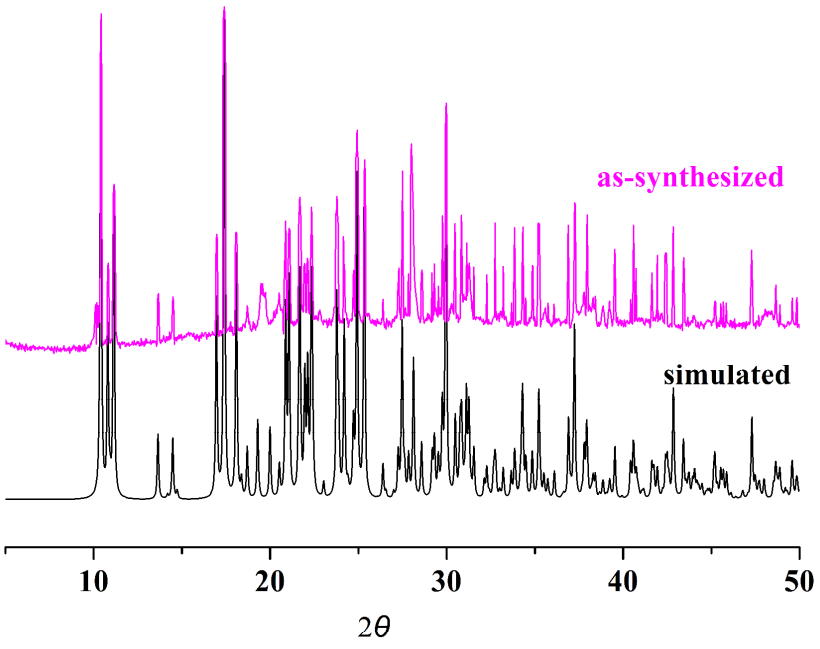

Figure S1. As-synthesized and simulated PXRD patterns of compound **1**.

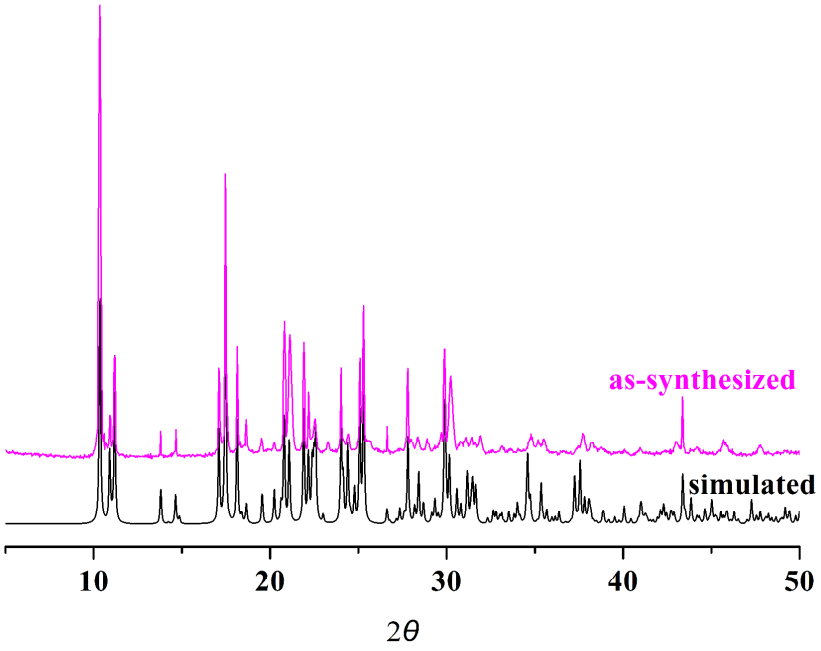

Figure S2. As-synthesized and simulated PXRD patterns of compound **2**.

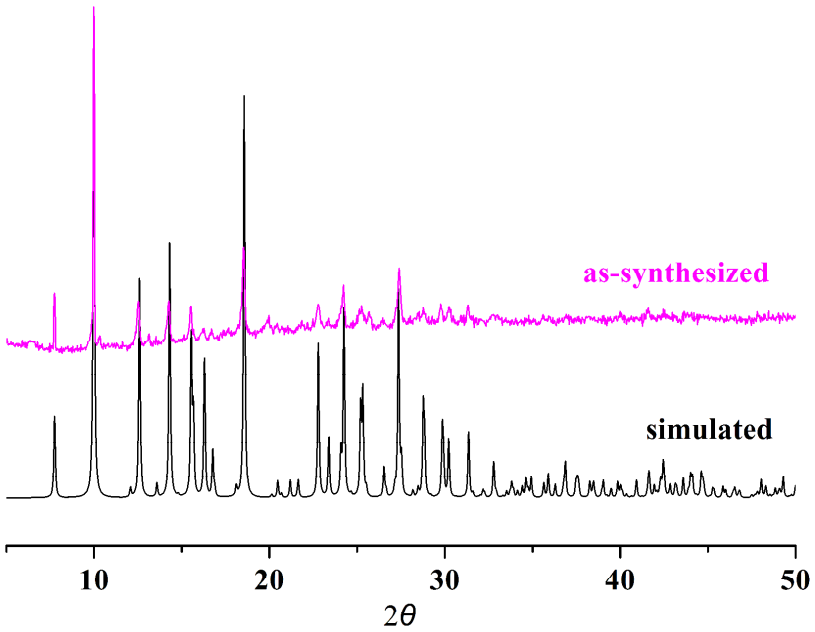

Figure S3. As-synthesized and simulated PXRD patterns of compound **3**.

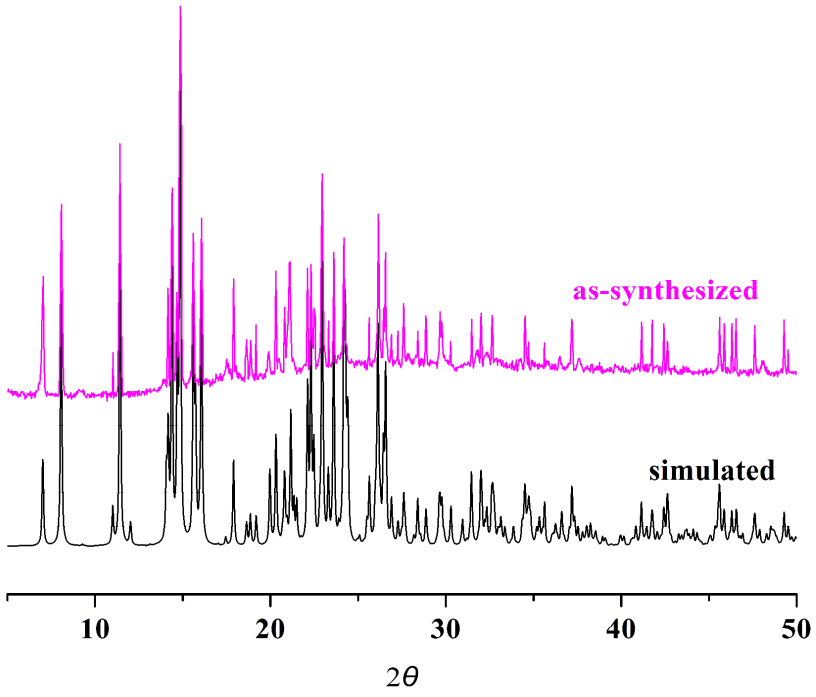

Figure S4. As-synthesized and simulated PXRD patterns of compound **4**.

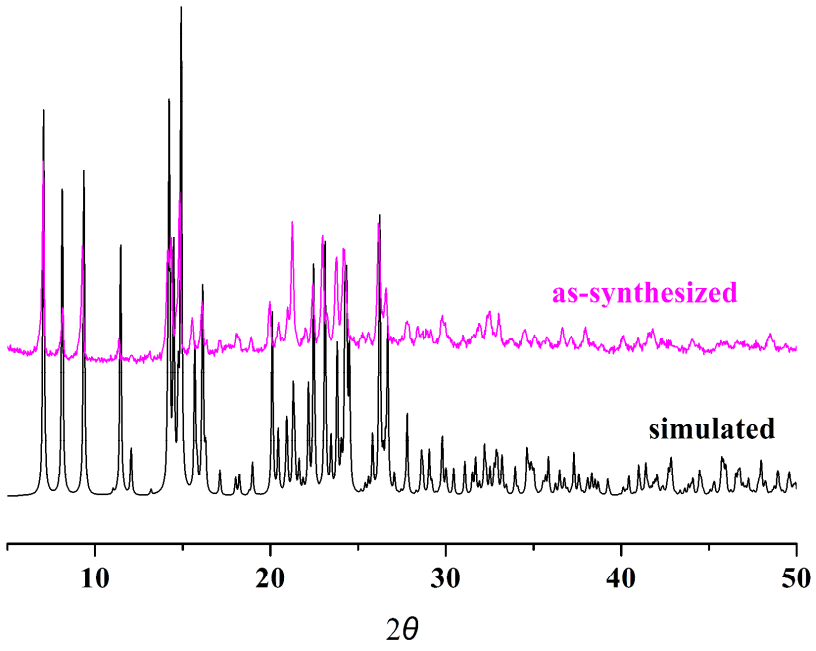

Figure S5. As-synthesized and simulated PXRD patterns of compound **5**.

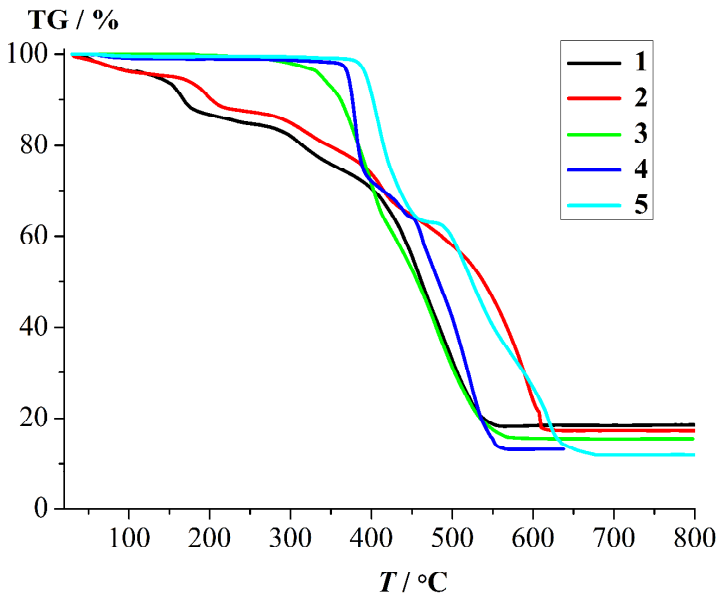

Figure S6. TGA curves of compounds **1**–**5**.

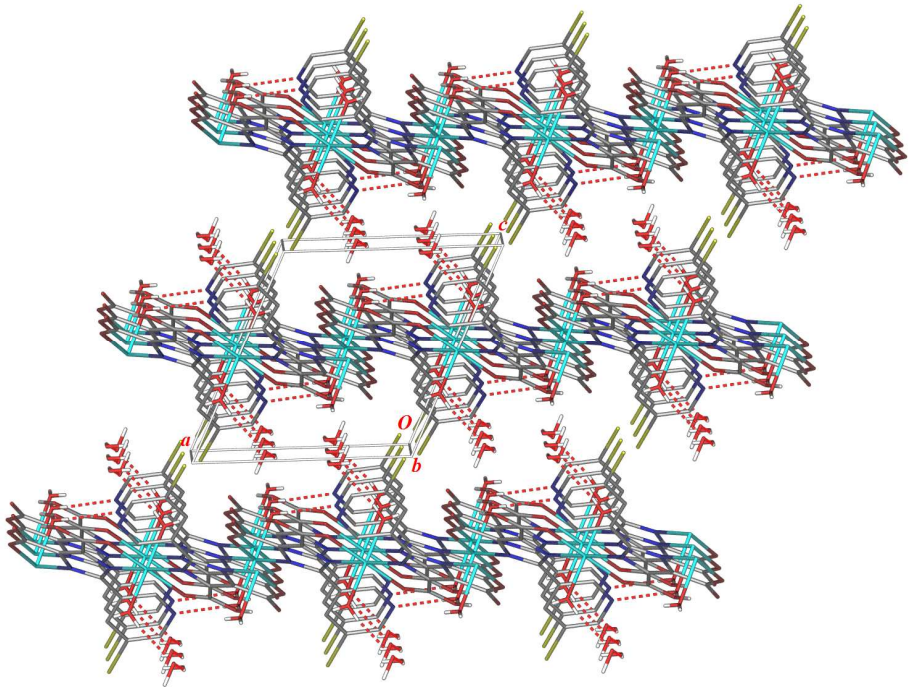

Figure S7. View of the stacking of 2D supramolecular frameworks in **1**, showing lattice water molecules being anchored between layers through hydrogen-bonding interactions.

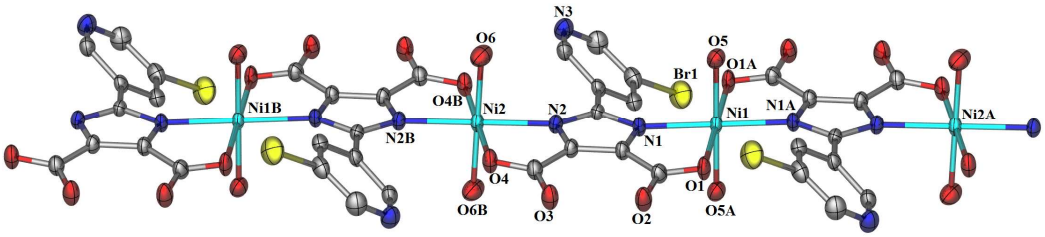

Figure S8. View of the typically linear chain structure in **2** formed by the imidazoledicarboxylates of $(HL)^{2-}$ ligands bis-chelating two independent Ni^{II}, showing the coordination environments of Ni1 and Ni2. Symmetry codes: (A) $-x$, $2-y$, $1-z$; (B) $1-x$, $1-y$, $1-z$.

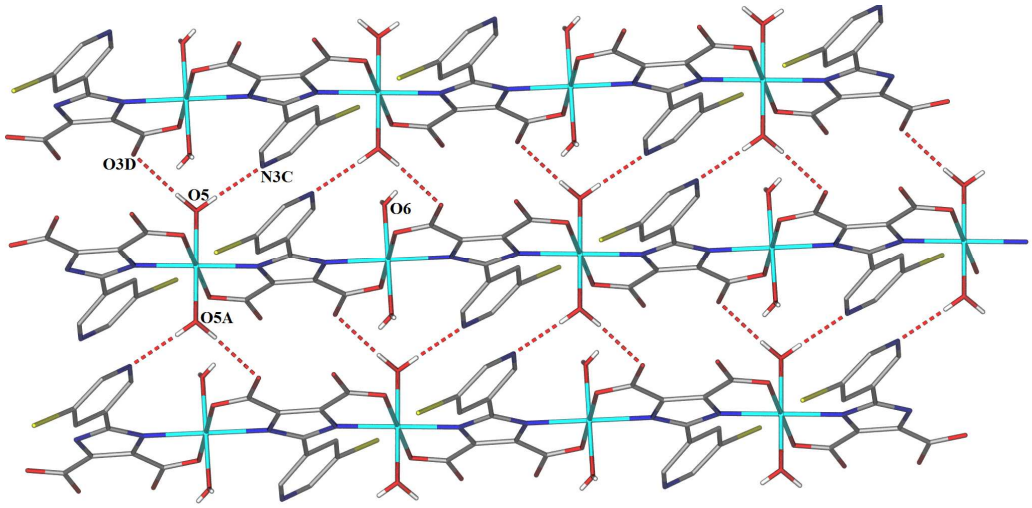

Figure S9. View of the 2D supramolecular framework of **2** formed by interchain hydrogen-bonding interactions. Symmetry codes: (A) $-x$, $2-y$, $1-z$; (C) $-1+x$, y, z; (D) $-x$, $1-y$, $1-z$.

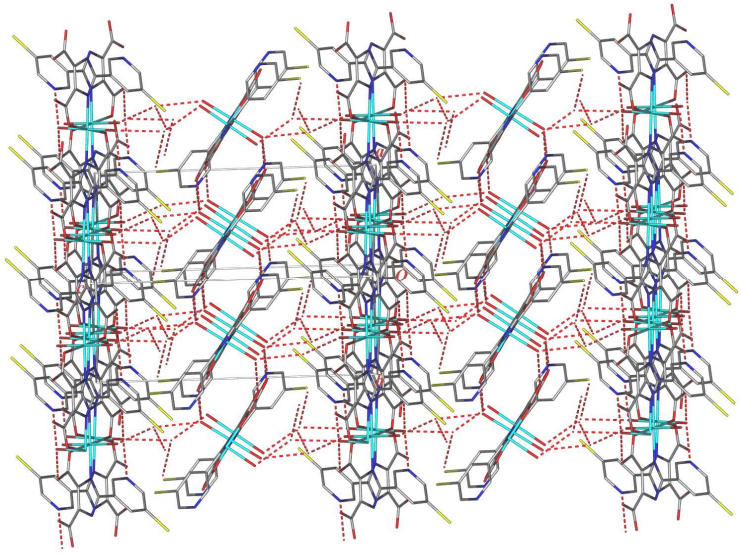

Figure S10. View of the stacking of 2D supramolecular frameworks in **2**, showing lattice water molecules being anchored between layers through hydrogen-bonding interactions.

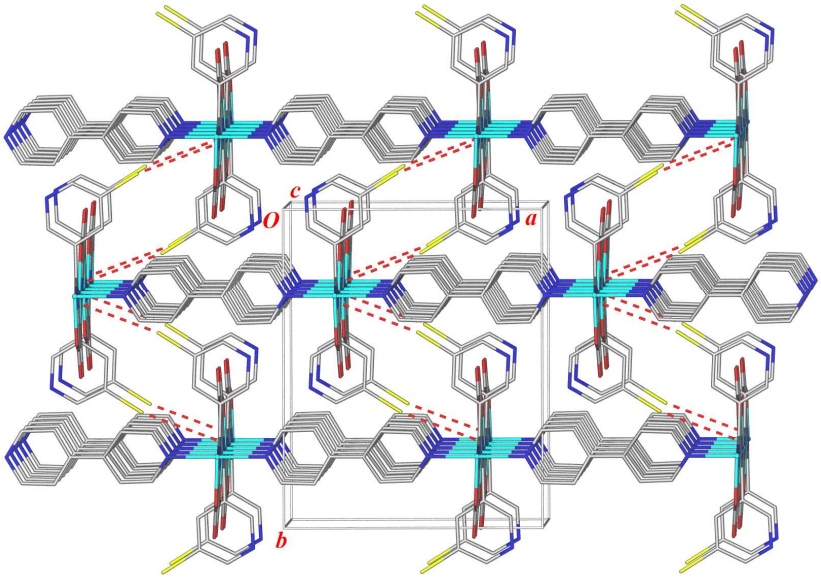

Figure S11. View of the 3D supramolecular framework of **3** formed through interlayered Br···π interactions.

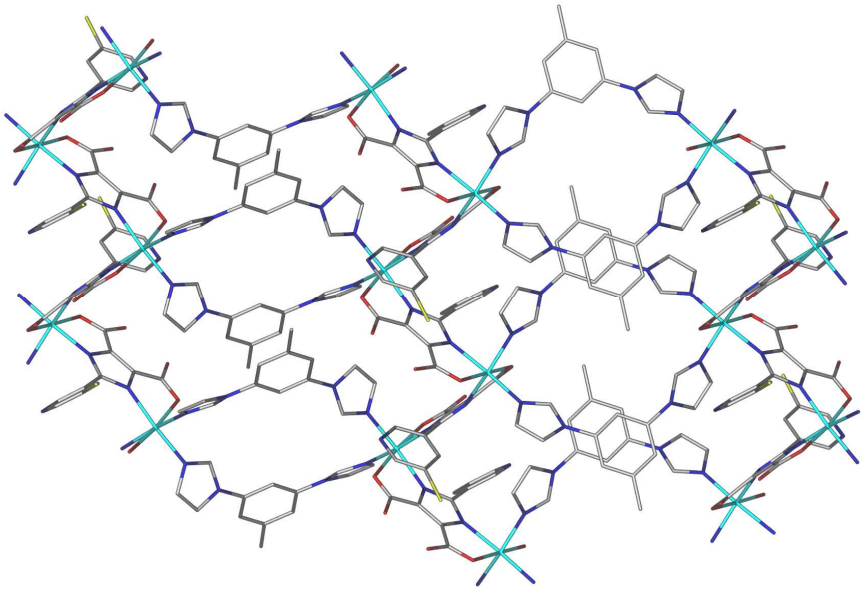

Figure S12. Helically constructed mesolayer in **4**, presenting an architecture with 6^3-topology as simplified the two doubly-bridged pbim ligands as one spacer.

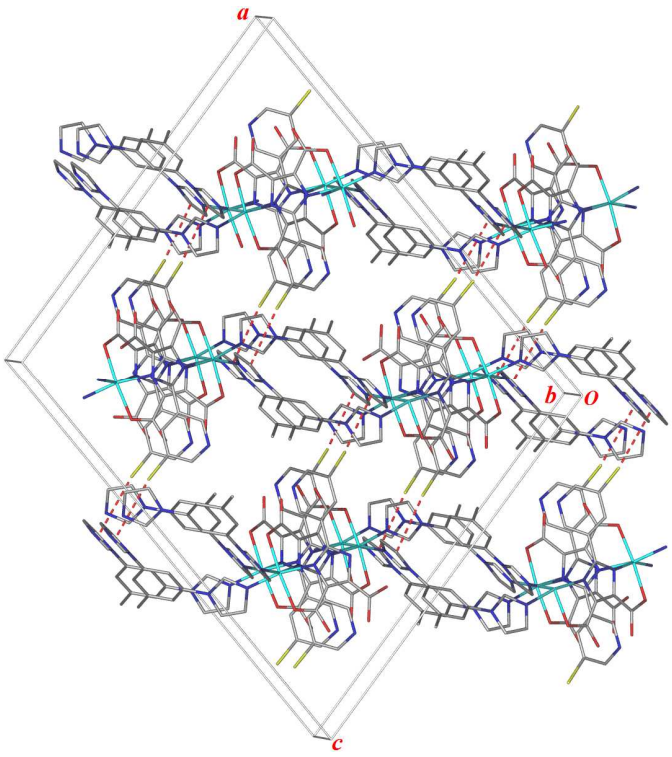

Figure S13. View of the 3D supramolecular framework of **4** formed through interlayered Br···π interactions.

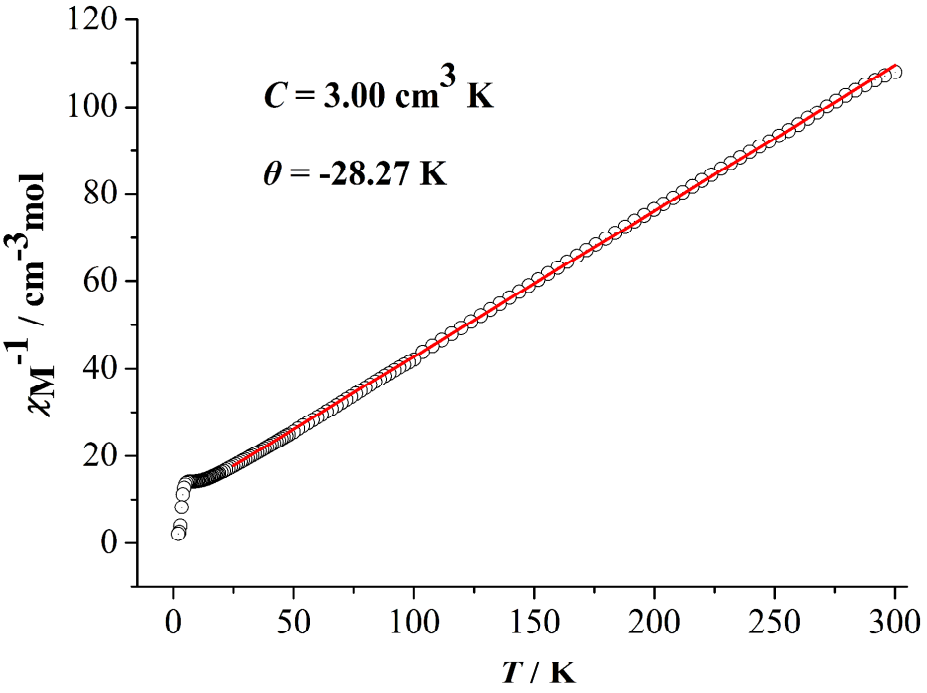

Figure S14. χ_M^{-1} vs T plot with the theoretical fit (—) for **1**.

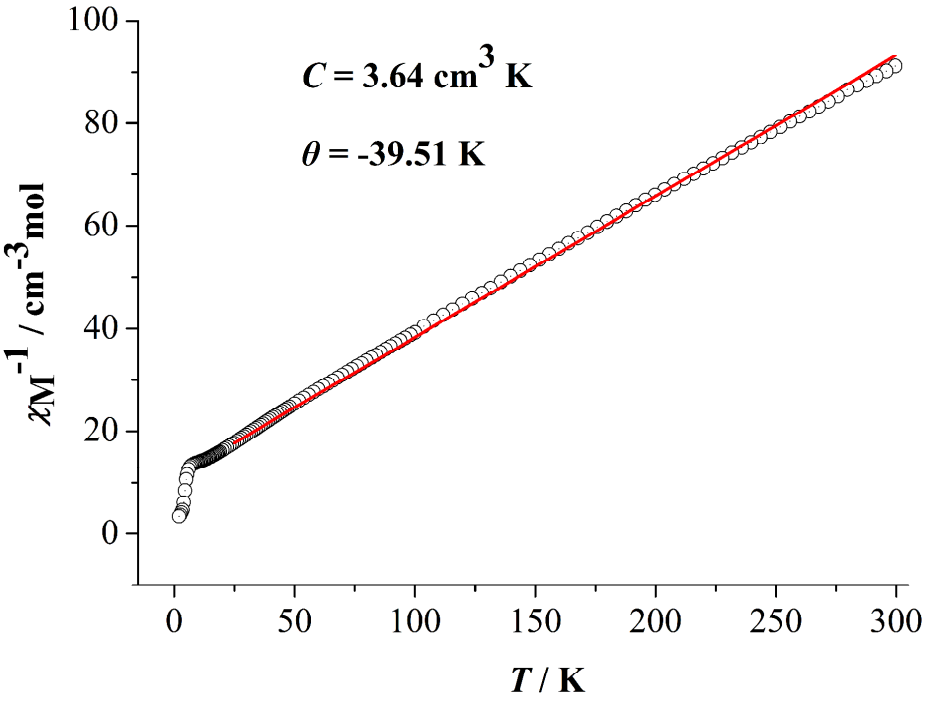

Figure S15. χ_M^{-1} vs T plot with the theoretical fit (—) for **3**.

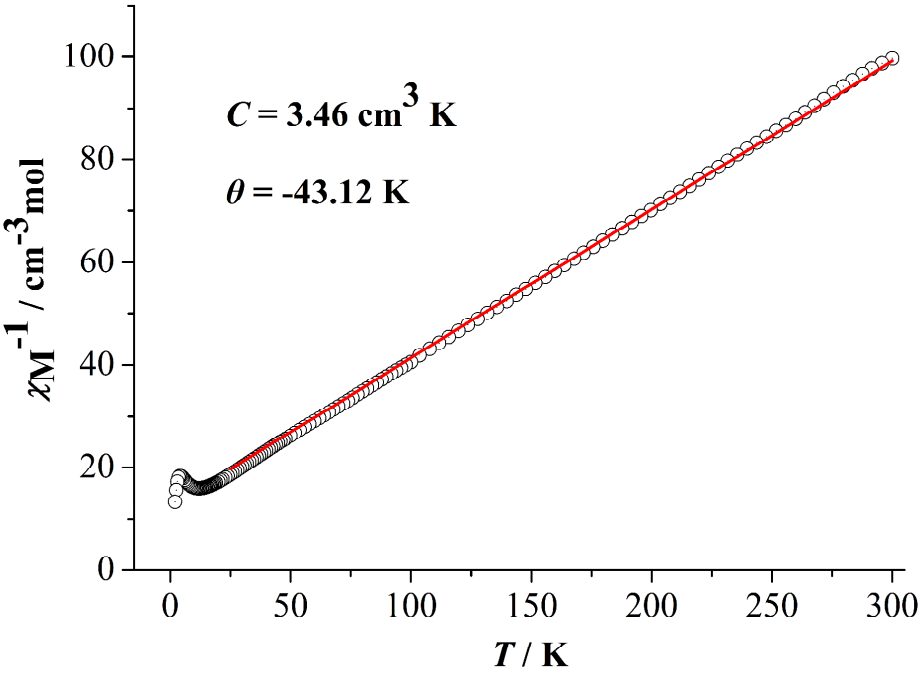

Figure S16. χ_M^{-1} vs T plot with the theoretical fit (—) for **4**.

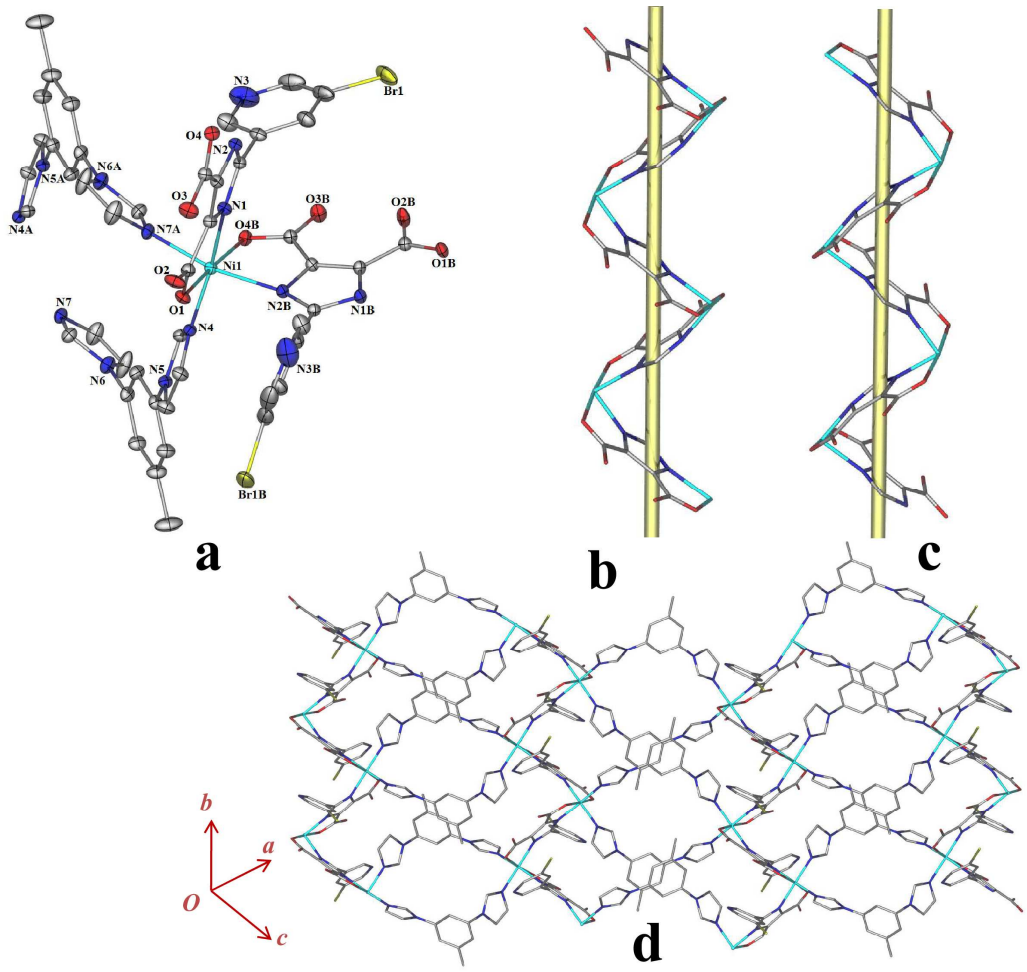

Figure S17. View of the coordination environment of Ni^{II} (a), *b* axially extended left- and right-handed helixes constructed by the imidazoledicarboxylates of $(HL)^{2-}$ ligands bis-chelating Ni^{II} ions with 5-bromo-pyridin-3-yl groups being omitted for clarity (b and c), and helically constructed mesolayer in **5** (d). Symmetry code: (A) − *x*, 1 − *y*, − *z*; (B) 1/2 − *x*, 1/2 + *y*, 1/2 − *z*.

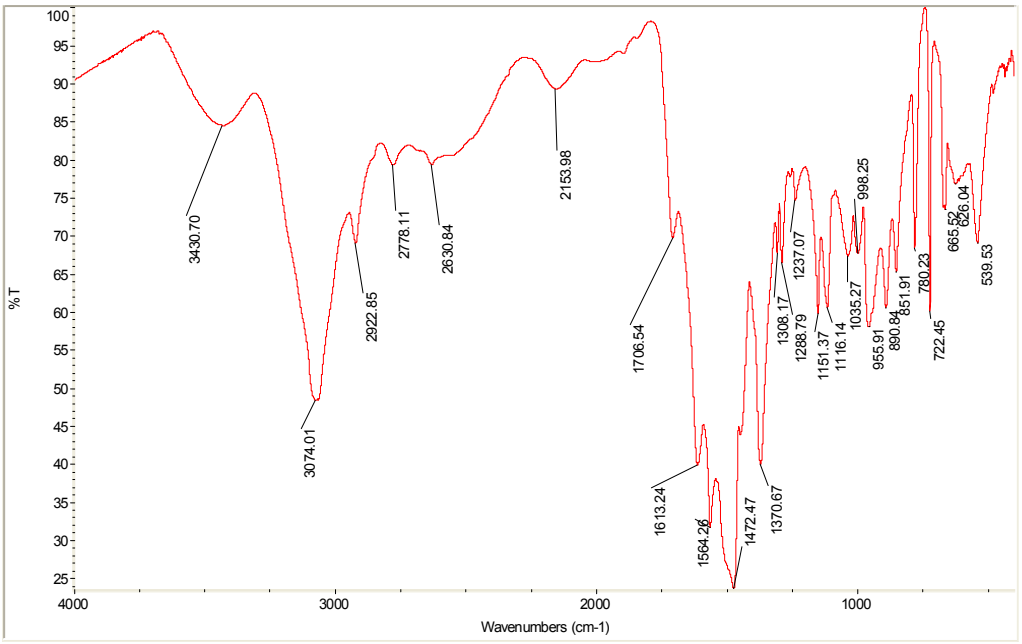

Figure S18. IR spectrum of free ligand H_3L.

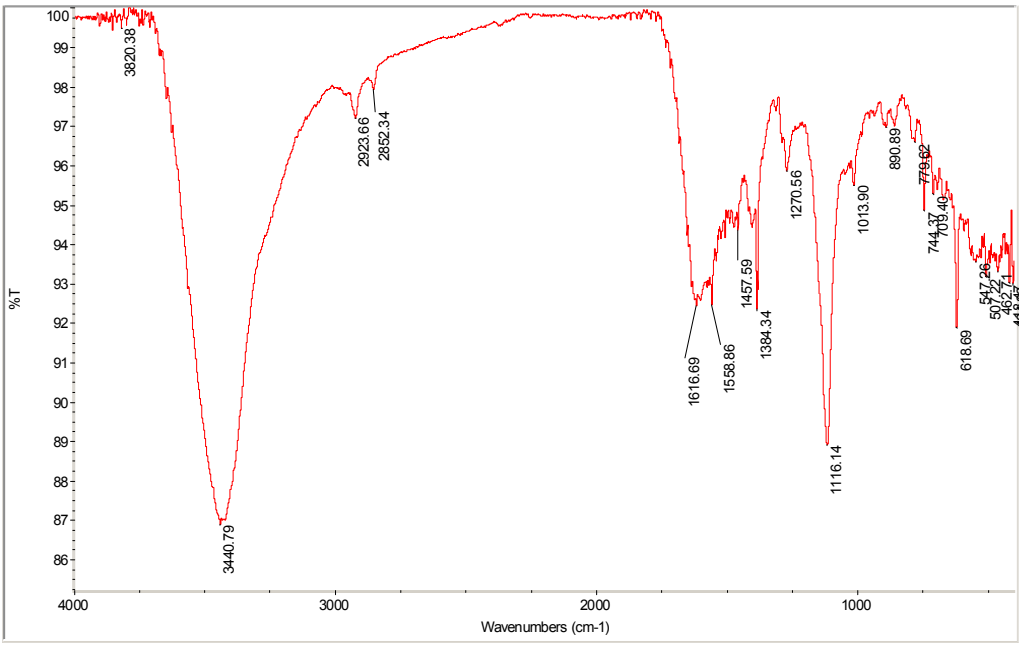

Figure S19. IR spectrum of compound **1**.

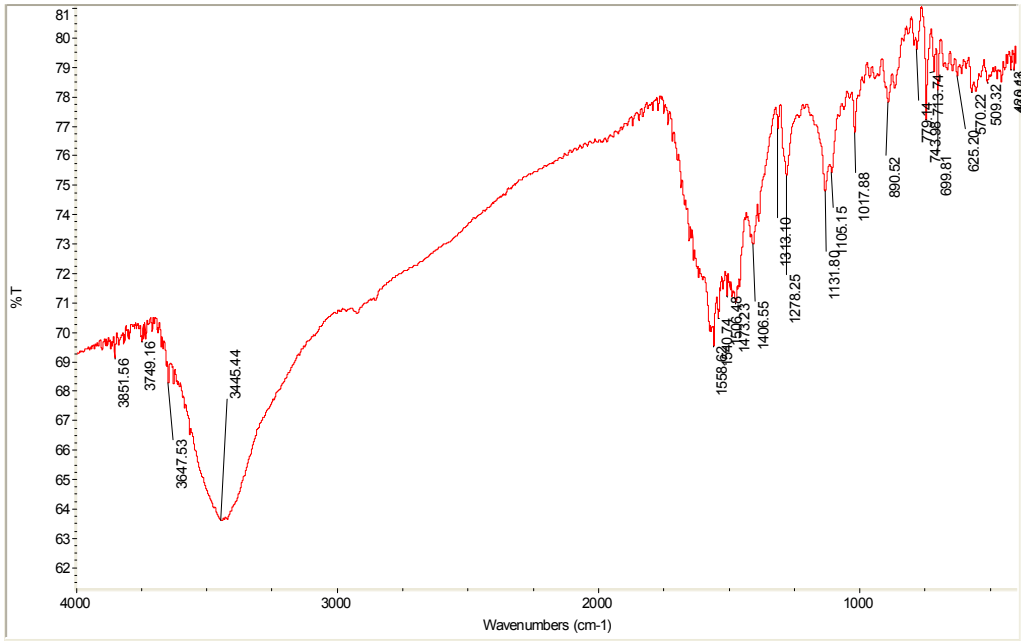

Figure S20. IR spectrum of compound **2**.

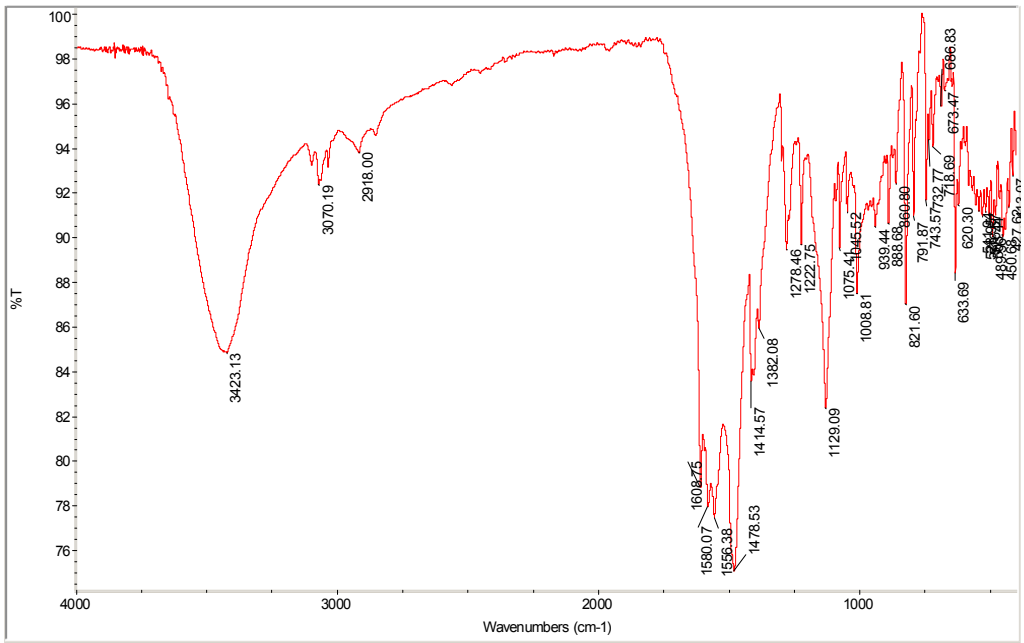

Figure S21. IR spectrum of compound **3**.

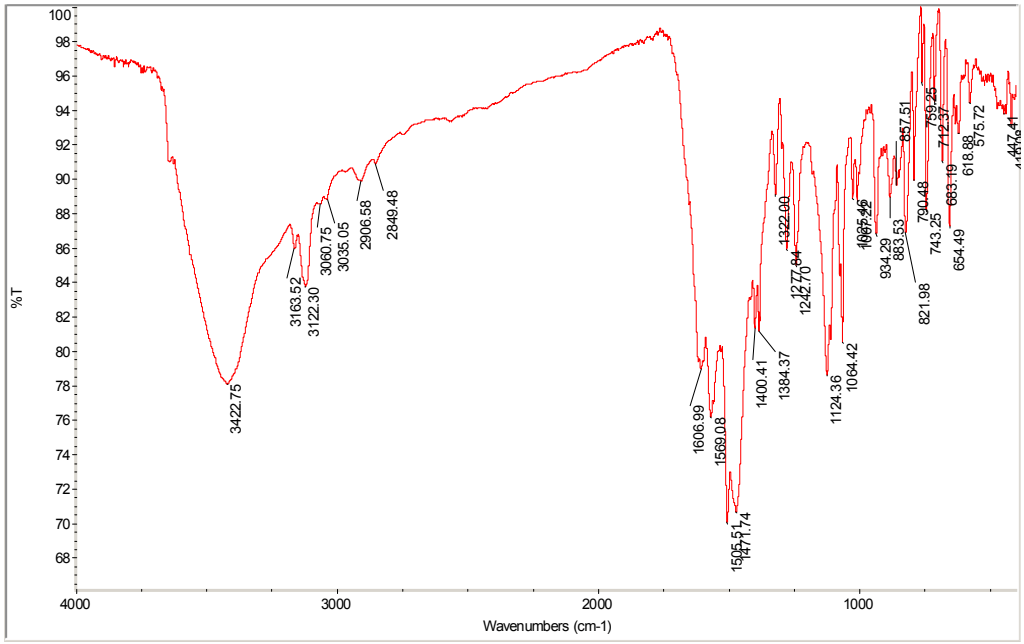

Figure S22. IR spectrum of compound **4**.

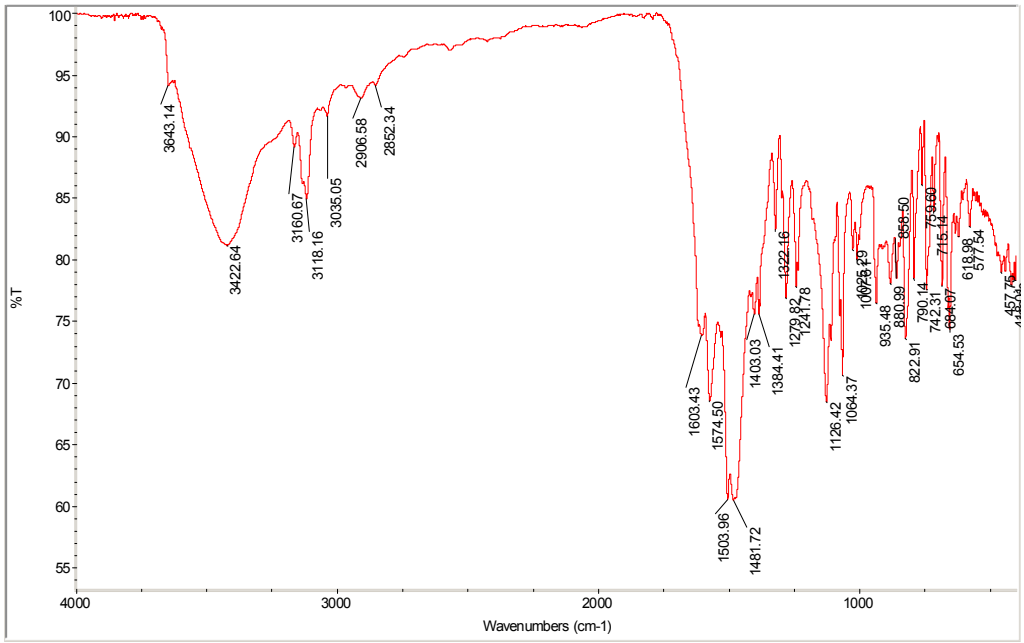

Figure S23. IR spectrum of compound **5**.