Supporting Information

Synthesis, structure and characterization of two new metal-organic coordination polymers based on the ligand 5-iodo-1, 3-benzenedicarboxylic acid

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FT-IR spectra

The FT-IR spectral data show features attributable to the carboxylate stretching vibrations of (**1**) and (**2**). The characteristic bands of the carboxylate groups appear in the range of 1622–1689 cm^{-1} for the asymmetric stretching and 1384–1521 cm^{-1} for the symmetric stretching, respectively. The broad band centred at 3400 cm^{-1} in **2** corresponds to the –OH stretching vibrations of the lattice water molecules.

PXRD Patterns

Powder X-ray diffraction analysis (PXRD) was used to check the phase purities of the complexes **1** and **2** (**Fig. S2, Fig. S3**). The PXRD patterns of the bulk samples **1** and **2** match very well with the corresponding simulated XRD patterns calculated from the single crystal data using Mercury 1.4.2 [http://www.ccdc.cam.ac.uk/Solutions/FreeSoftware/Pages/FreeMercury.aspx], indicating the high phase purities of the products **1** and **2**.

Figure 1

PXRD patterns for **1** recorded (black) the simulated XRD pattern calculated from single-crystal data with Mercury 1.4.2, (red) the sample as-synthesized.

Figure 2

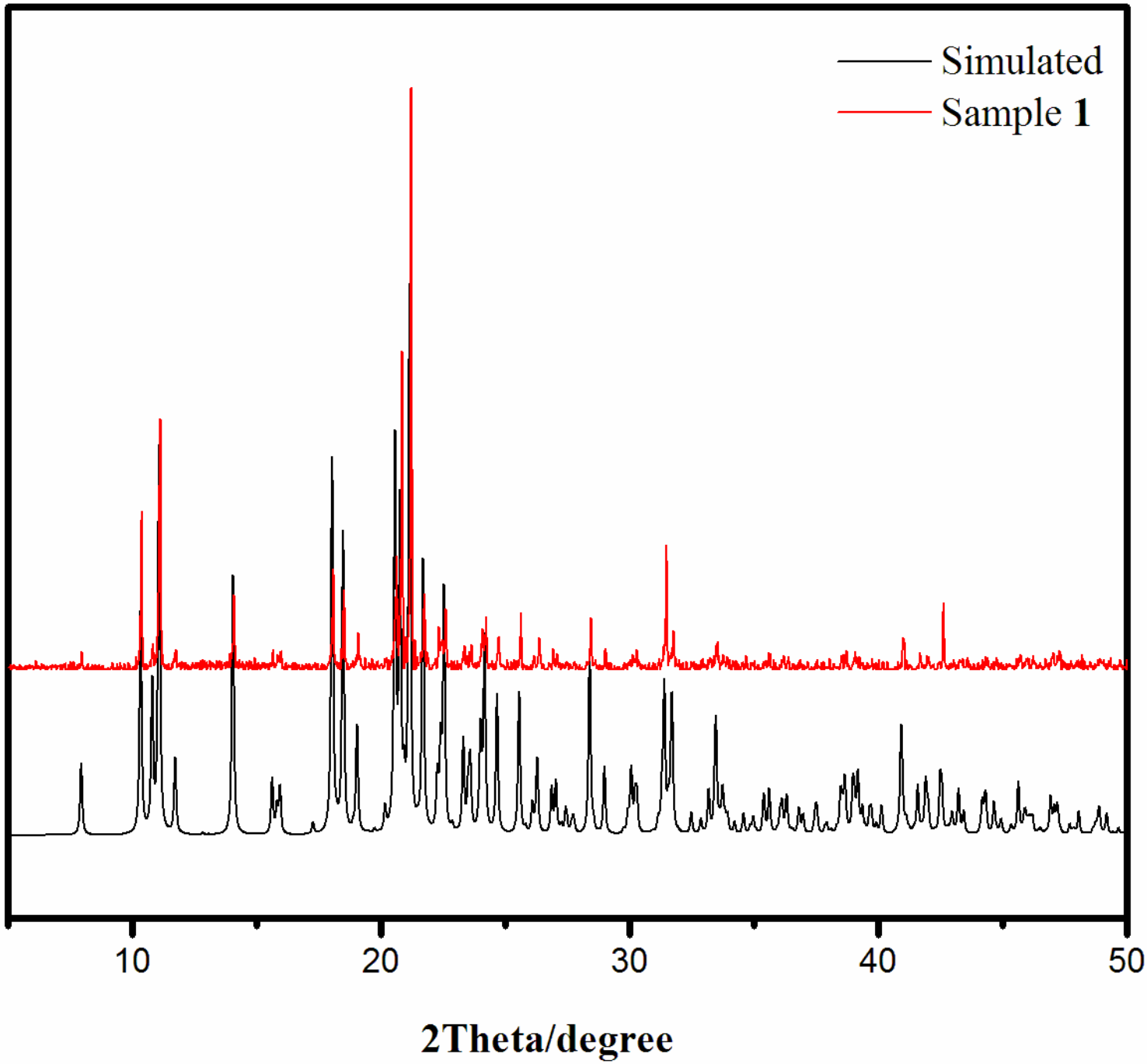
PXRD patterns for **2** recorded (black) the simulated XRD pattern calculated from single-crystal data with Mercury 1.4.2, (red) the sample as-synthesized.

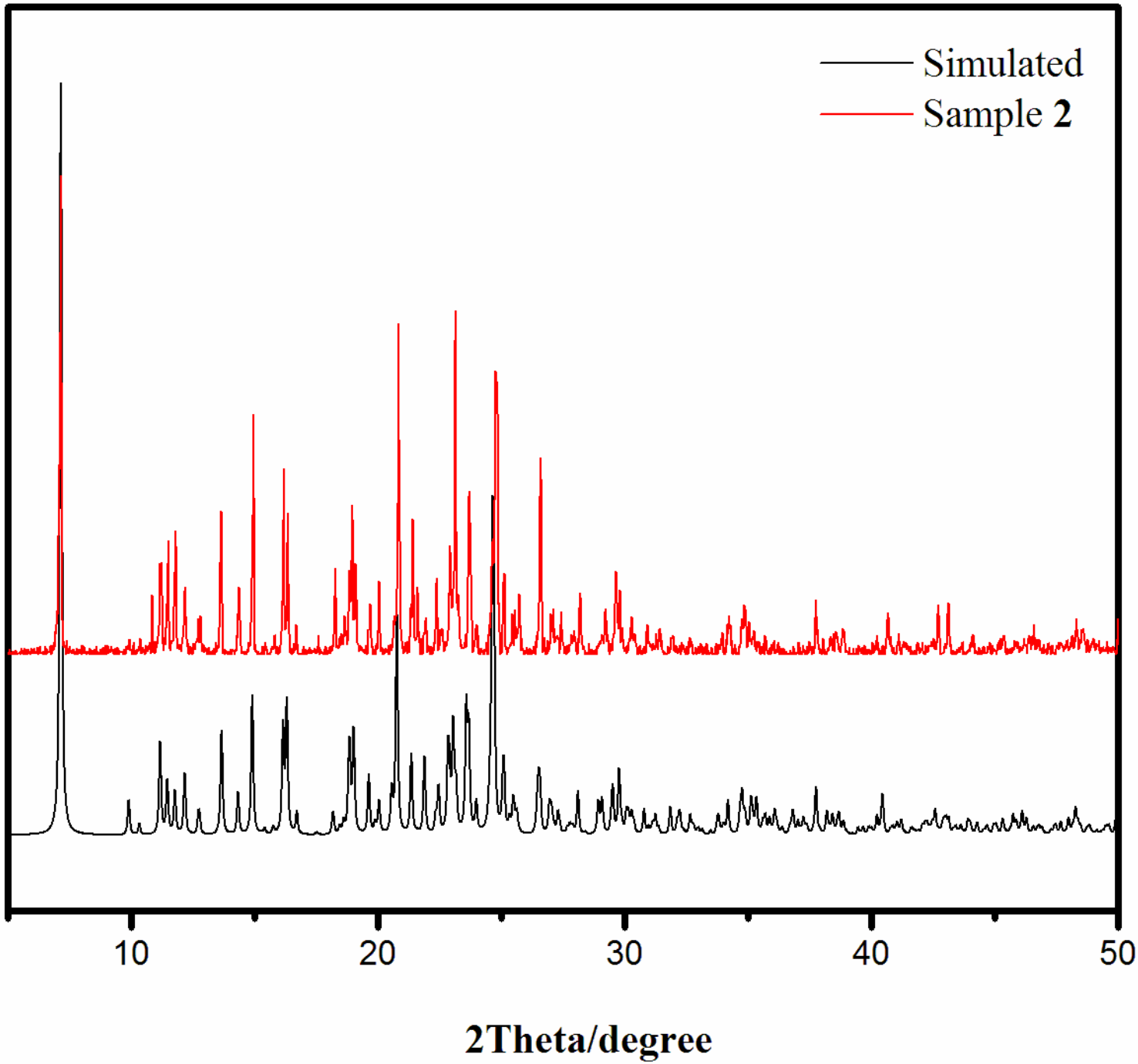
Figure S3

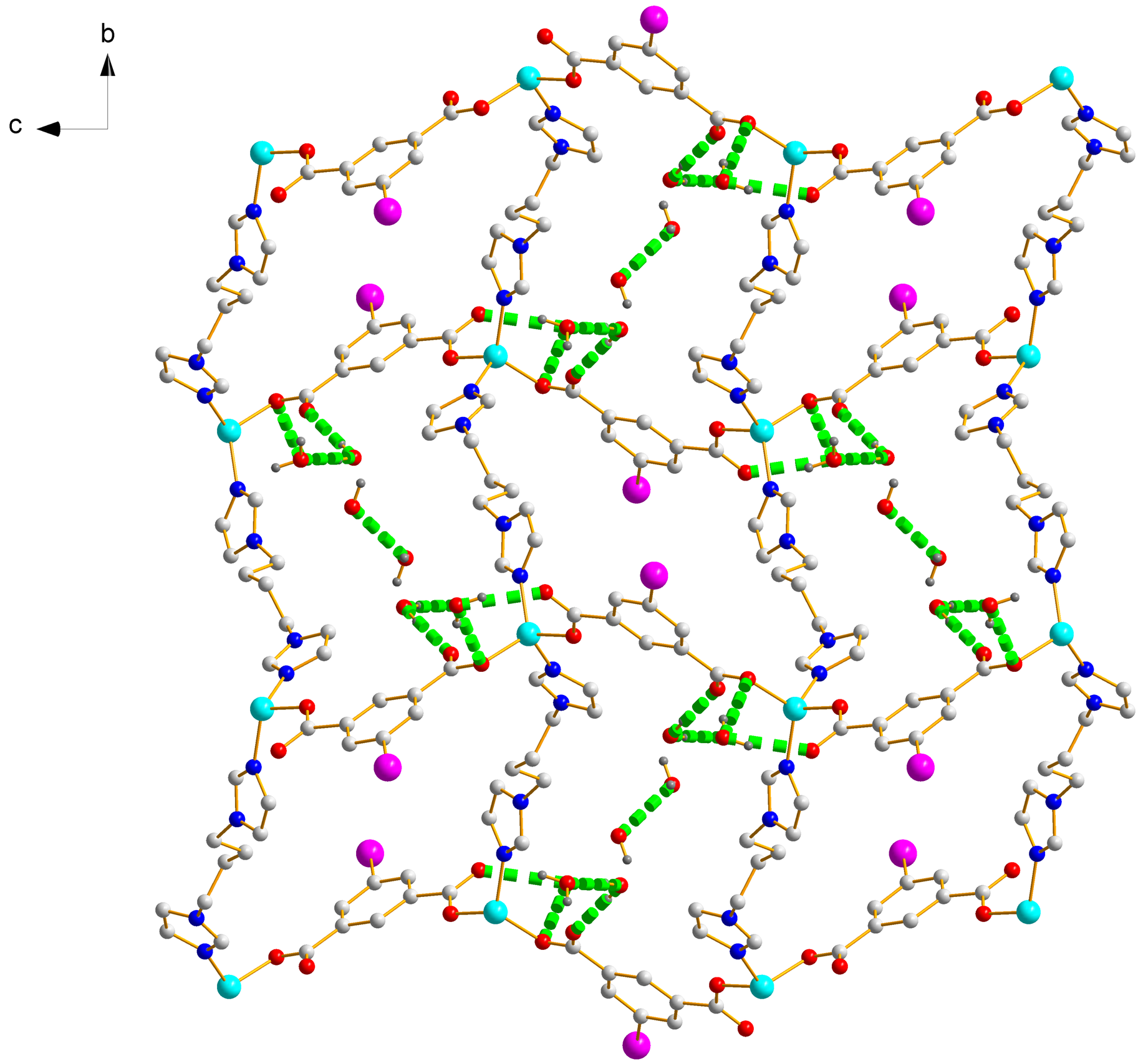
2D layered network along [100] direction with 1D channel formed through the interlayer hydrogen bonds.

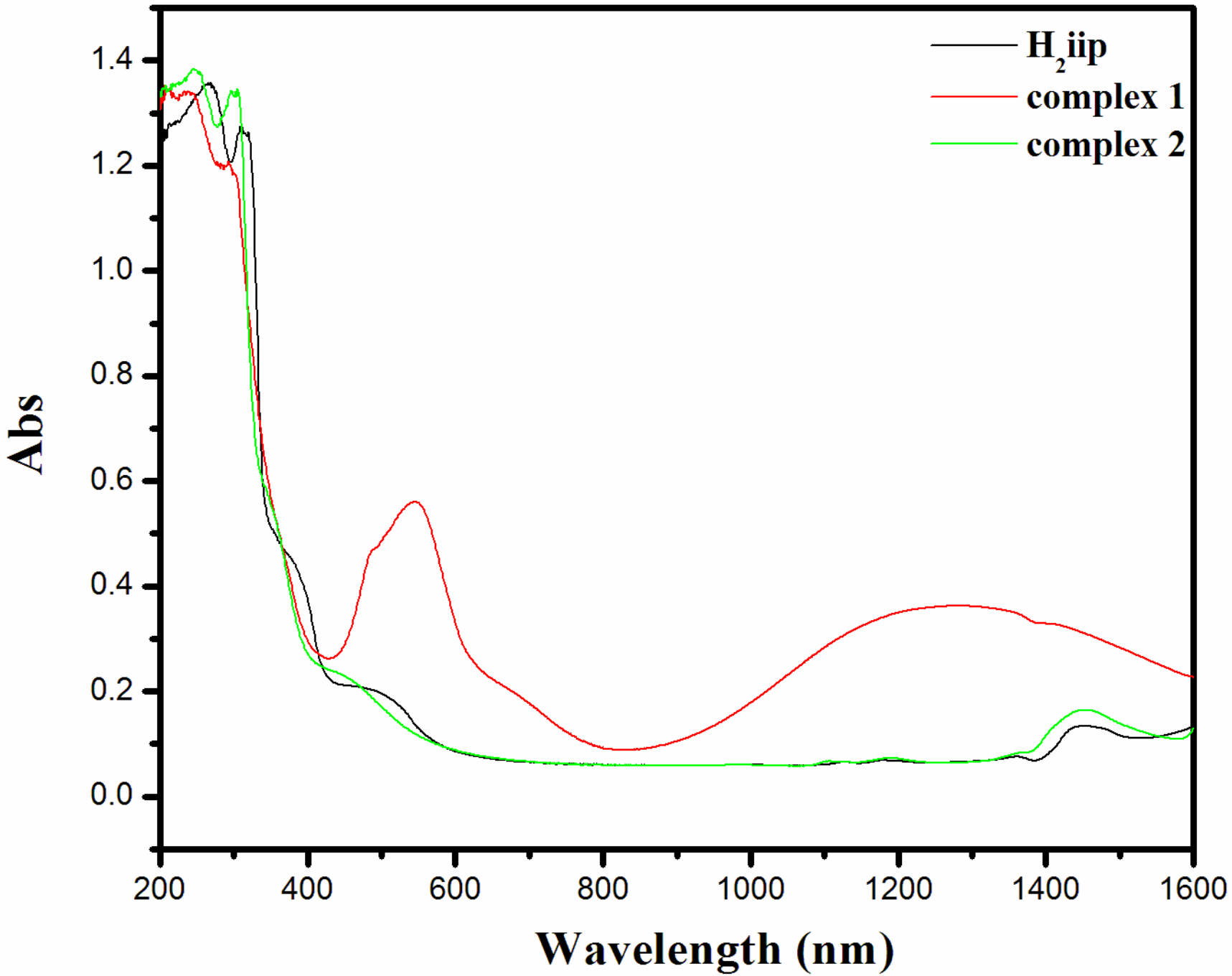
Figure S4

The solid state UV–Vis absorption spectra for H_2iip (black), **1** (red) and **2** (green).


Simulated
Sample 1
10
20
30
40
50
2Theta/degree


Simulated
Sample 2
10
20
30
40
50
2Theta/degree


b
c


H2iip
complex 1
complex 2
Abs
Wavelength (nm)
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
200
400
600
800
1000
1200
1400
1600