Supporting information

Lone Pair-π Interaction-induced Generation of Non-interpenetrated and Photochromic Cuboid 3-D Naphthalene Diimide Coordination Networks

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1. Single Crystal Structures

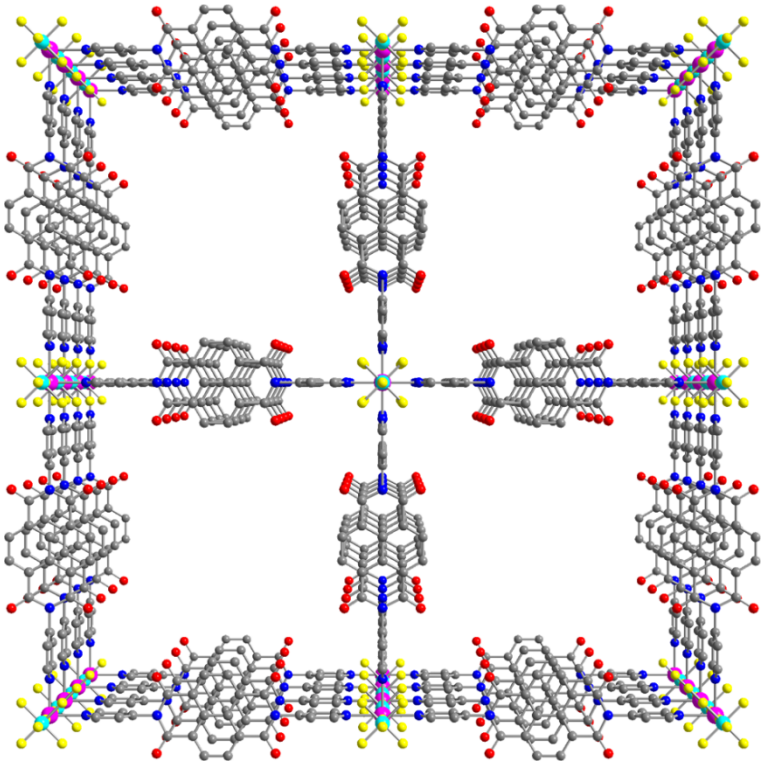

Figure S1. Perspective view of three-dimensional framework of **1** with 1-D channels along the *c*-axis

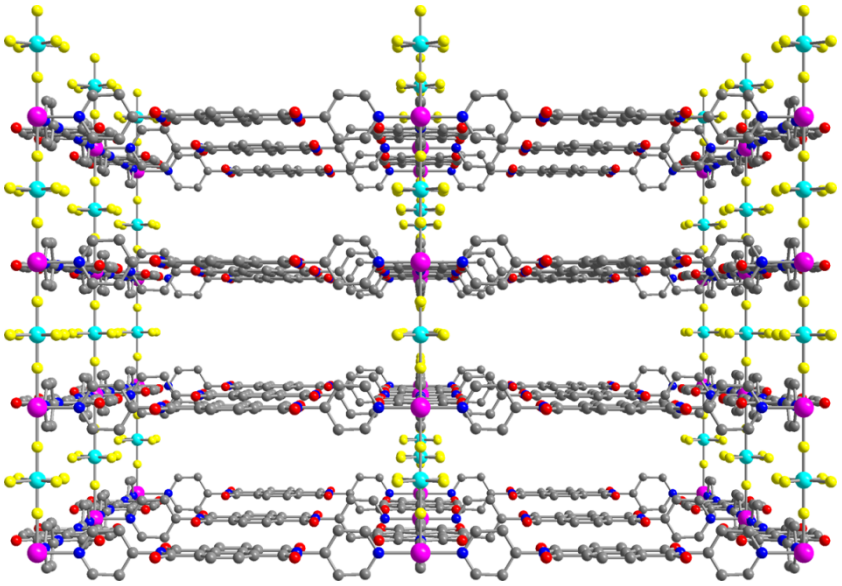

Figure S2. Perspective view of Three-dimensional framework of **1** along the *b*-axis

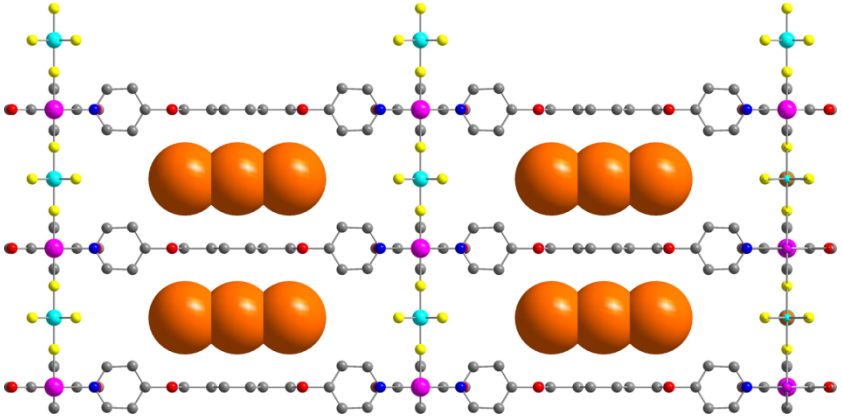

Figure S3. The I_2 molecules filled in the framework of **2** viewed along the *b*-axis (I_2 molecules with respective *ca.* 40% occupancies at both antipodal imide units for each DPNDI unit in the mezzanines)

Table S1. Selected bond lengths (Å) for **1**

Bonds	**Dist. (Å)**	**Bonds**	**Dist. (Å)**
Zn(1)-F(2)	2.009(3)	Zn(1)-F(2)#1	2.009(3)
Zn(1)-N(1)#2	2.154(3)	Zn(1)-N(1)#1	2.154(3)
Zn(1)-N(1)	2.154(3)	Zn(1)-N(1)#3	2.154(3)
Si(1)-F(1)#4	1.660(2)	Si(1)-F(1)#5	1.660(2)
Si(1)-F(1)	1.660(2)	Si(1)-F(1)#3	1.660(2)
Si(1)-F(2)#4	1.706(3)	Si(1)-F(2)	1.706(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1, -y+1, -z+1; #2 y, -x+1, -z+1; #3 -y+1, x, z; #4 -x+1, -y+1, -z; #5 y, -x+1, -z.

Table S2. Selected bond lengths (Å) for **2**

Bonds	**Dist. (Å)**	**Bonds**	**Dist. (Å)**
Zn(1)-F(1)	2.030(5)	Zn(1)-F(1)#1	2.030(5)
Zn(1)-N(1)#2	2.163(5)	Zn(1)-N(1)#3	2.163(5)
Zn(1)-N(1)#1	2.163(5)	Zn(1)-N(1)	2.163(5)
I(1)-I(2)	2.809(4)	I(2)-I(1)#4	2.809(4)
Si(1)-F(2)	1.670(4)	Si(1)-F(2)#5	1.670(4)
Si(1)-F(2)#6	1.670(4)	Si(1)-F(2)#3	1.670(4)
Si(1)-F(1)#5	1.708(5)	Si(1)-F(1)	1.708(5)

Symmetry transformations used to generate equivalent atoms:

#1 -x, -y, -z; #2 y, -x, -z; #3 -y, x, z; #4 -x+1, -y, -z-1; #5 -x, -y, -z+1; #6 y, -x, -z+1.

2. X-ray Powder Diffraction

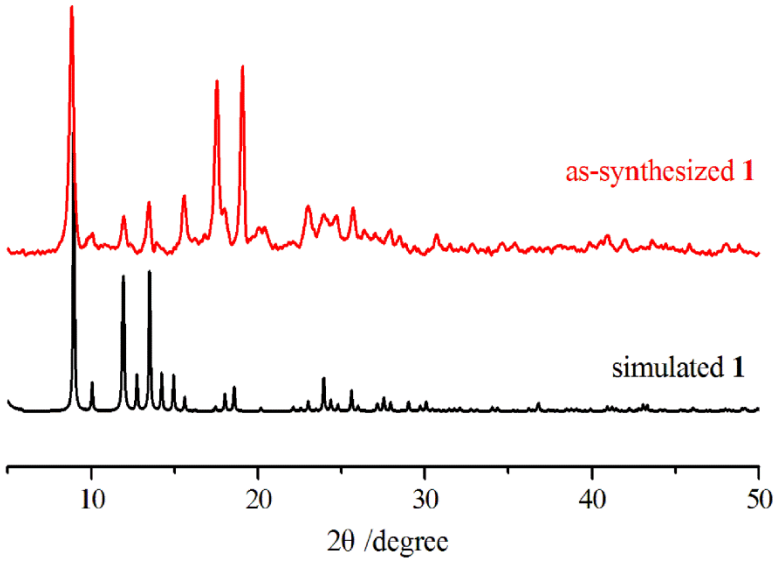

Figure S4. Comparison of the simulated and synthesized PXRD for **1**.

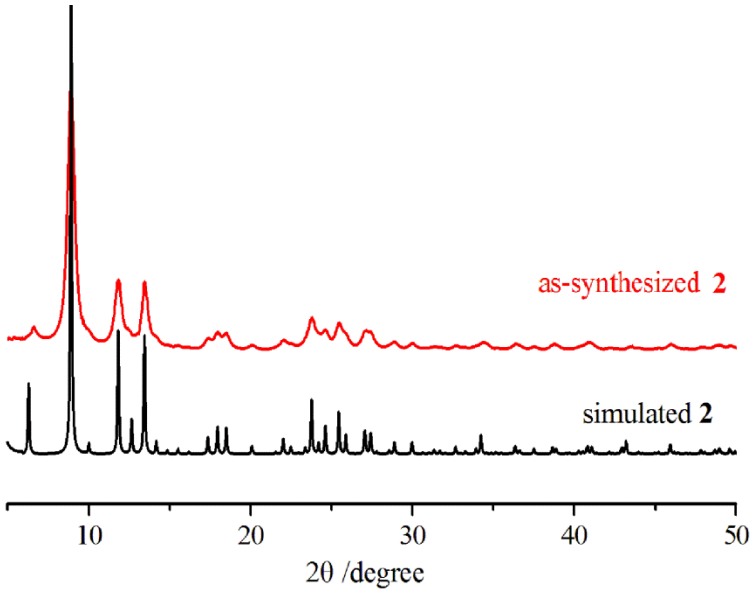

Figure S5. Comparison of the simulated and synthesized PXRD for **2**.

3. Thermogravimetric analyses

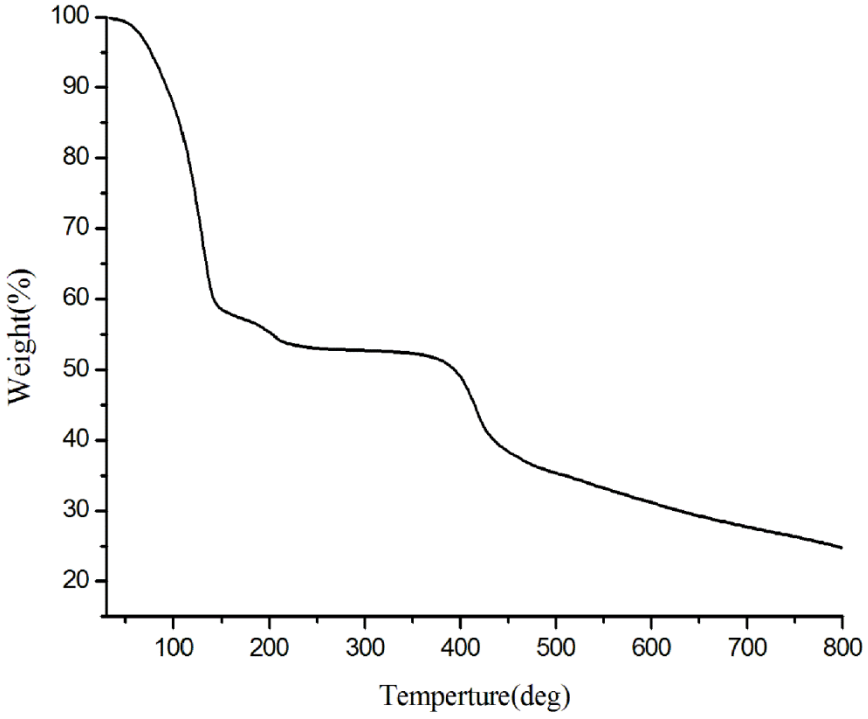

Figure S6. TGA pattern of the complex **1**.

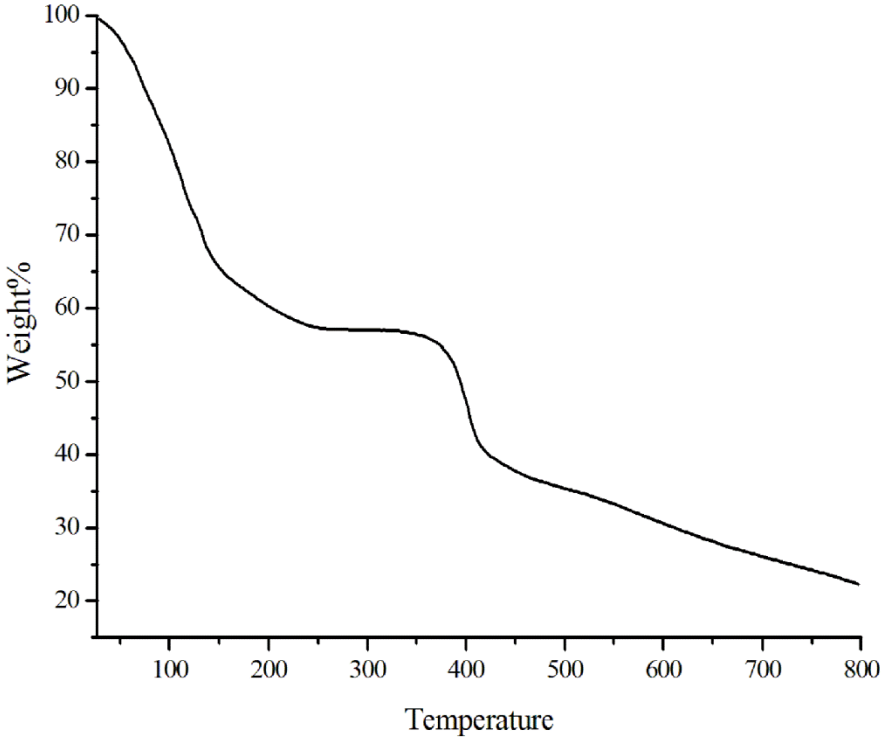

Figure S7. TGA pattern of the complex **2**.

4. IR Studies

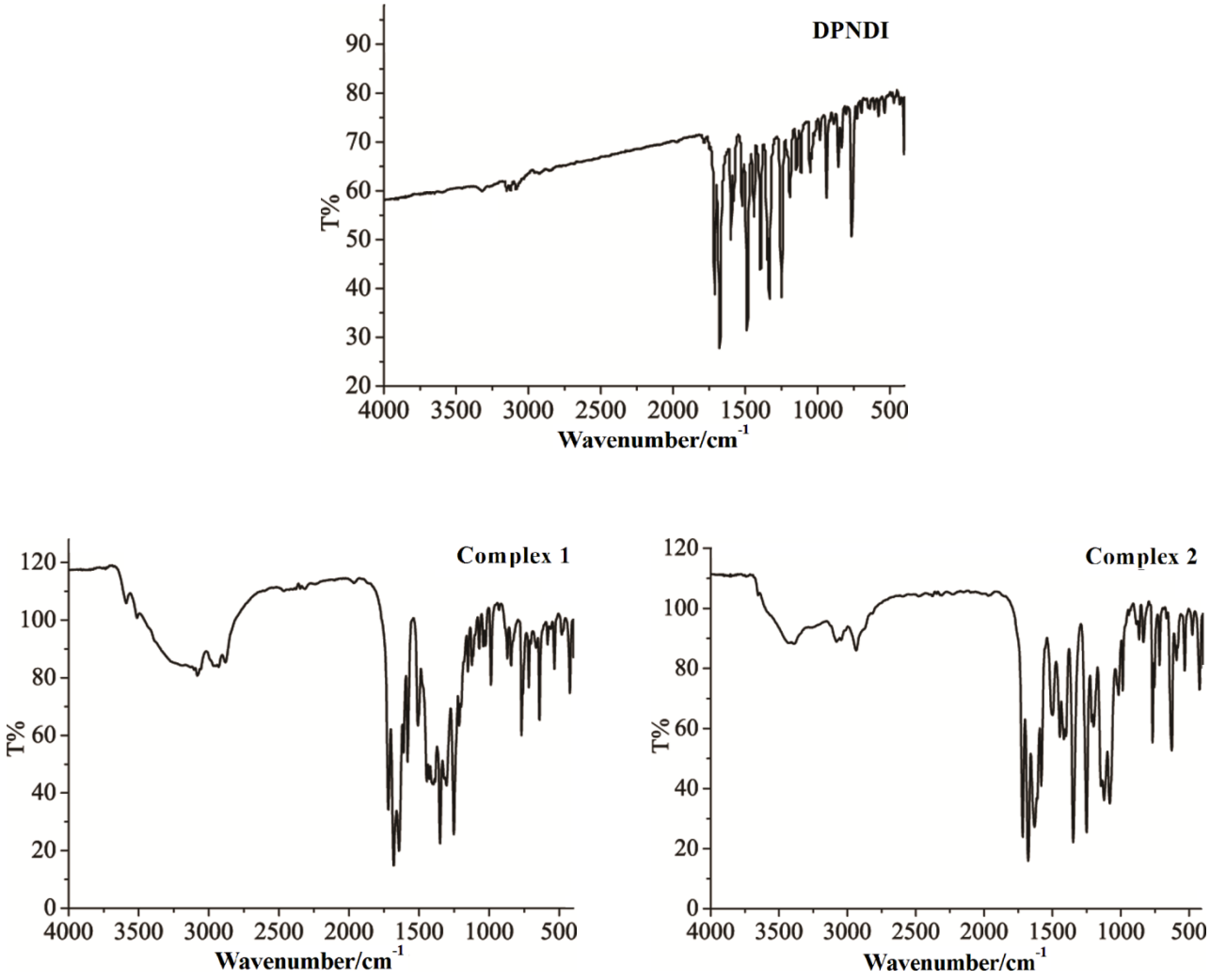

Figure S8. IR spectra of DPNDI, **1** and **2**.