Electronic Supplementary Material (ESI) for Dalton Transactions.

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# A Naphthalene Diimide-based Metal-organic Framework as

## An Electron-deficient Platform with Photochromic and

### **Chemochromic Properties**

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Fig. S1 The asymmetric unit of 1@DMF (symmetry codes: A: x, 0.5-y, -0.5+z; B: 2-x,



Fig. 2 Thermo-gravimetric (TG) and Differential scanning calorimetry (DSC) curves of



1@DMF.

Fig. S3 TG curve of 1 and 1-Adsorbing DMF.



Fig. S4 Powder X-ray diffraction (PXRD) patterns for 1@DMF, 1 and 1-Adsorbing



DMF at room temperature.

Fig. S5 The UV-vis absorption spectra and switching cycles of coloration-

decoloration processes of 1@DMF (477nm) upon alternating UV light illumination



Fig. S6 IR spectra of 1@DMF, 1@DMF-P and 1@DMF-P-80 °C.



Fig. S7 UV-vis absorption spectra of 1.



Fig. S8 EPR spectra of 1 and 1P.



Fig. S9 The XPS core-level spectra of 1 and 1P before and after UV light irradiation at

room temperature.



Fig. S10 TG spectra of 1@DMA, 1@DMSO, 1@NMP and 1-Adsorbing DMF.



Fig. S11 UV-Vis absorption spectra (a), EPR spectra (b) and PXRD spectra (c) of

1@amines (amines=AN, TEOA, DIP, TEA).

#### 2. Tables

 Table S1. Crystallographic data and refinement of 1@DMF.

Compounds	1@DMF
CCDC code	2052963
Temperature (K)	273(2)
Empirical formula	$C_{34}H_{35}N_5O_9Zn$
Formula weight	723.04
Crystal size (mm)	0.673 × 0.398 × 0.078
Crystal system	monoclinic
Space group	P21/c
<i>a</i> (Å)	10.4323(13)
b (Å)	19.699(3)
<i>c</i> (Å)	17.150(2)
α (°)	90
β (°)	101.046(3)
γ (°)	90
V (ų)	3459.1(7)
Ζ	4
D <sub>c</sub> (g cm <sup>-3</sup> )	1.388
F(000)	1504.0
μ(mm <sup>-1</sup> )	0.771
Reflections collected	50746
Independent reflections	8609
R <sub>int</sub>	0.0232
Goodness-of-fit on F <sup>2</sup>	1.074
$R_1/wR_2$ , $[I \ge 2\sigma(I)]^{a,b}$	0.0406/ 0.1243
$R_1/wR_2$ , (all data)	0.0536/ 0.1399

$\begin{array}{c ccccccccccccccccccccccccccccccccccc$			1@DMF	
Zn(1)-O(3)         2.0313(14)         C(13)-C(12)#6         1.399(4)           Zn(1)-O(4)#1         2.0454(15)         C(14)-C(15)         1.505(2)           Zn(1)-O(5)#2         2.0434(14)         C(15)-C(16)         1.410(3)           Zn(1)-O(6)#3         2.0442(14)         C(15)-C(16)         1.410(3)           Zn(1)-O(6)#3         2.0442(14)         C(15)-C(16)         1.420(3)           O(1)-C(7)         1.206(4)         C(17)-C(18)         1.420(3)           O(2)-C(8)         1.214(3)         C(18)-C(24)         1.415(3)           O(3)-C(14)         1.256(3)         C(18)-C(24)         1.416(3)           O(4)-C(14)         1.250(3)         C(19)-C(21)         1.416(3)           O(4)-C(14)         1.250(3)         C(12)-C(22)         1.361(3)           O(5)-C(1)##1         2.0453(14)         C(21)-C(22)         1.361(3)           O(5)-C(25)         1.258(3)         C(22)-C(23)         1.412(3)           O(6)-C(7)         1.258(3)         C(23)-C(24)         1.370(3)           O(6)-C(15)         1.339(3)         N(3)-C(26)         1.442(7)           N(1)-C(5)         1.339(3)         N(3)-C(27)         1.375(5)           N(2)-C(6)         1.476(3)         N(3)-C(27)         1.34	Zn(1)-Zn(1) #1	2.9684(5)	C(12)-C(13)#6	1.398(4)
Zn(1)-O(4)#1         2.0434(14)         C(14)-C(15)         1.505(2)           Zn(1)-O(5)#2         2.0434(14)         C(15)-C(16)         1.410(3)           Zn(1)-O(6)#3         2.0442(14)         C(15)-C(20)         1.370(3)           Zn(1)-N(1)         2.0319(18)         C(16)-C(17)         1.363(3)           O(1)-C(7)         1.206(4)         C(17)-C(18)         1.420(3)           O(2)-C(8)         1.214(3)         C(18)-C(19)         1.415(3)           O(3)-C(14)         1.256(3)         C(19)-C(20)         1.416(3)           O(4)-C(14)         1.250(3)         C(19)-C(21)         1.419(3)           O(5)-Zn(1)#4         2.0435(14)         C(21)-C(22)         1.361(3)           O(5)-C(25)         1.258(3)         C(22)-C(23)         1.412(3)           O(6)-C(25)         1.251(3)         C(23)-C(25)         1.501(2)           N(1)-C(1)         1.332(3)         O(7)-C(28)         1.202(7)           N(1)-C(5)         1.339(3)         N(3)-C(25)         1.442(7)           N(2)-C(6)         1.476(3)         N(3)-C(28)         1.341(6)           N(2)-C(7)         1.394(4)         N(3)-C(28)         1.341(6)           N(2)-C(6)         1.373(4)         N(4)-C(30)         1.351(8)	Zn(1)-O(3)	2.0313(14)	C(13)-C(12)#6	1.399(4)
Zn(1)-O(5)#2         2.0434(14)         C(15)-C(16)         1.410(3)           Zn(1)-O(6)#3         2.0442(14)         C(15)-C(20)         1.370(3)           Zn(1)-N(1)         2.0319(18)         C(16)-C(17)         1.363(3)           O(1)-C(7)         1.206(4)         C(17)-C(18)         1.420(3)           O(2)-C(8)         1.214(3)         C(18)-C(19)         1.415(3)           O(3)-C(14)         1.256(3)         C(18)-C(21)         1.415(3)           O(4)-Zn(1)#1         2.0435(14)         C(19)-C(21)         1.419(3)           O(5)-Zn(1)#4         2.0435(14)         C(12)-C(22)         1.361(3)           O(5)-Zn(1)#4         2.0435(14)         C(21)-C(22)         1.361(3)           O(5)-C(25)         1.258(3)         C(22)-C(23)         1.412(3)           O(6)-C(25)         1.251(3)         C(23)-C(24)         1.370(3)           O(6)-C(25)         1.251(3)         C(23)-C(25)         1.501(2)           N(1)-C(1)         1.332(3)         O(7)-C(28)         1.242(7)           N(1)-C(1)         1.332(3)         O(8)-C(31)         1.248(9)           C(1)-C(7)         1.394(4)         N(3)-C(28)         1.341(6)           N(2)-C(6)         1.366(4)         N(4)-C(30)         1.351(8)	Zn(1)-O(4)#1	2.0454(15)	C(14)-C(15)	1.505(2)
Zn(1)-O(6)#3       2.0442(14)       C(15)-C(20)       1.370(3)         Zn(1)-N(1)       2.0319(18)       C(16)-C(17)       1.363(3)         O(1)-C(7)       1.206(4)       C(17)-C(18)       1.420(3)         O(2)-C(8)       1.214(3)       C(18)-C(19)       1.415(3)         O(3)-C(14)       1.256(3)       C(18)-C(24)       1.415(3)         O(4)-Zn(1)#1       2.0453(14)       C(19)-C(21)       1.419(3)         O(4)-C(14)       1.250(3)       C(19)-C(21)       1.419(3)         O(5)-Zn(1)#4       2.0435(14)       C(21)-C(22)       1.361(3)         O(6)-Zn(1)#5       2.0441(14)       C(23)-C(24)       1.370(3)         O(6)-C(25)       1.258(3)       C(22)-C(23)       1.412(3)         O(6)-C(25)       1.251(3)       C(23)-C(25)       1.501(2)         N(1)-C(1)       1.332(3)       O(7)-C(28)       1.202(7)         N(1)-C(1)       1.332(3)       O(7)-C(28)       1.202(7)         N(1)-C(5)       1.339(3)       N(3)-C(26)       1.442(7)         N(2)-C(6)       1.476(3)       N(3)-C(28)       1.341(6)         N(2)-C(7)       1.339(4)       N(3)-C(28)       1.341(6)         N(2)-C(3)       1.379(5)       N(4)-C(29)       1.430(7)	Zn(1)-O(5)#2	2.0434(14)	C(15)-C(16)	1.410(3)
Zn(1)-N(1)         2.0319(18)         C(16)-C(17)         1.363(3)           O(1)-C(7)         1.206(4)         C(17)-C(18)         1.420(3)           O(2)-C(8)         1.214(3)         C(18)-C(19)         1.415(3)           O(3)-C(14)         1.256(3)         C(18)-C(24)         1.415(3)           O(4)-Zn(1)#1         2.0453(14)         C(19)-C(20)         1.416(3)           O(4)-C(14)         1.250(3)         C(19)-C(21)         1.419(3)           O(5)-Zn(1)#4         2.0435(14)         C(21)-C(22)         1.361(3)           O(5)-C(25)         1.258(3)         C(22)-C(23)         1.412(3)           O(6)-C(25)         1.251(3)         C(23)-C(24)         1.370(3)           O(6)-C(1)#5         2.0441(14)         C(23)-C(25)         1.501(2)           N(1)-C(1)         1.332(3)         O(7)-C(28)         1.202(7)           N(1)-C(1)         1.332(3)         O(7)-C(28)         1.341(6)           N(2)-C(6)         1.476(3)         N(3)-C(26)         1.442(7)           N(2)-C(7)         1.394(4)         N(3)-C(28)         1.341(6)           N(2)-C(8)         1.337(3)         O(8)-C(31)         1.358(8)           C(1)-C(2)         1.373(4)         N(4)-C(30)         1.351(8) <td>Zn(1)-O(6)#3</td> <td>2.0442(14)</td> <td>C(15)-C(20)</td> <td>1.370(3)</td>	Zn(1)-O(6)#3	2.0442(14)	C(15)-C(20)	1.370(3)
O(1)-C(7)         1.206(4)         C(17)-C(18)         1.420(3)           O(2)-C(8)         1.214(3)         C(18)-C(19)         1.415(3)           O(3)-C(14)         1.256(3)         C(18)-C(24)         1.415(3)           O(4)-Zn(1)#1         2.0453(14)         C(19)-C(20)         1.416(3)           O(4)-Cn(1)#4         2.0455(14)         C(19)-C(21)         1.419(3)           O(5)-Zn(1)#4         2.0435(14)         C(21)-C(22)         1.361(3)           O(5)-C(25)         1.258(3)         C(22)-C(23)         1.412(3)           O(6)-C(25)         1.251(3)         C(23)-C(24)         1.370(3)           O(6)-C(25)         1.251(3)         C(23)-C(24)         1.370(3)           O(6)-C(25)         1.323(3)         O(7)-C(28)         1.202(7)           N(1)-C(1)         1.332(3)         O(7)-C(28)         1.341(6)           N(2)-C(6)         1.476(3)         N(3)-C(26)         1.442(7)           N(2)-C(7)         1.394(4)         N(3)-C(28)         1.341(6)           N(2)-C(7)         1.394(4)         N(3)-C(28)         1.341(6)           N(2)-C(7)         1.373(4)         N(4)-C(30)         1.351(8)           C(1)-C(2)         1.379(5)         N(4)-C(30)         1.351(8)	Zn(1)-N(1)	2.0319(18)	C(16)-C(17)	1.363(3)
O(2)-C(8)         1.214(3)         C(18)-C(19)         1.415(3)           O(3)-C(14)         1.256(3)         C(18)-C(24)         1.415(3)           O(4)-Zn(1)#1         2.0453(14)         C(19)-C(20)         1.416(3)           O(4)-C(14)         1.250(3)         C(19)-C(21)         1.419(3)           O(5)-Zn(1)#4         2.0435(14)         C(21)-C(22)         1.361(3)           O(5)-C(25)         1.258(3)         C(22)-C(23)         1.412(3)           O(6)-Zn(1)#5         2.0441(14)         C(23)-C(24)         1.370(3)           O(6)-C(25)         1.251(3)         C(23)-C(25)         1.501(2)           N(1)-C(1)         1.332(3)         O(7)-C(28)         1.202(7)           N(1)-C(5)         1.339(3)         N(3)-C(26)         1.442(7)           N(2)-C(6)         1.476(3)         N(3)-C(28)         1.341(6)           N(2)-C(7)         1.394(4)         N(3)-C(28)         1.341(6)           N(2)-C(7)         1.394(4)         N(4)-C(30)         1.351(8)           C(1)-C(2)         1.373(4)         N(4)-C(30)         1.351(8)           C(3)-C(4)         1.366(4)         N(4)-C(33)         1.426(7)           C(4)-C(5)         1.383(3)         O(9)-C(33)         1.427(8)	O(1)-C(7)	1.206(4)	C(17)-C(18)	1.420(3)
O(3)-C(14)         1.256(3)         C(18)-C(24)         1.415(3)           O(4)-Zn(1)#1         2.0453(14)         C(19)-C(20)         1.416(3)           O(4)-C(14)         1.250(3)         C(19)-C(21)         1.419(3)           O(5)-Zn(1)#4         2.0435(14)         C(21)-C(22)         1.361(3)           O(5)-C(25)         1.258(3)         C(22)-C(23)         1.412(3)           O(6)-C(25)         1.251(3)         C(23)-C(25)         1.501(2)           N(1)-C(1)         1.332(3)         O(7)-C(28)         1.202(7)           N(1)-C(1)         1.332(3)         O(7)-C(28)         1.202(7)           N(1)-C(1)         1.332(3)         O(7)-C(28)         1.341(6)           N(2)-C(6)         1.476(3)         N(3)-C(27)         1.375(5)           N(2)-C(7)         1.394(4)         N(3)-C(28)         1.341(6)           N(2)-C(7)         1.394(4)         N(3)-C(28)         1.341(6)           N(2)-C(3)         1.379(5)         N(4)-C(30)         1.351(8)           C(3)-C(4)         1.366(4)         N(4)-C(31)         1.367(6)           C(4)-C(5)         1.383(3)         O(9)-C(33)         1.426(7)           C(4)-C(6)         1.506(4)         N(5)-C(32)         1.468(8)	O(2)-C(8)	1.214(3)	C(18)-C(19)	1.415(3)
O(4)-Zn(1)#1         2.0453(14)         C(19)-C(20)         1.416(3)           O(4)-C(14)         1.250(3)         C(19)-C(21)         1.419(3)           O(5)-Zn(1)#4         2.0435(14)         C(21)-C(22)         1.361(3)           O(5)-C(25)         1.258(3)         C(22)-C(23)         1.412(3)           O(6)-Zn(1)#5         2.0441(14)         C(23)-C(24)         1.370(3)           O(6)-C(25)         1.251(3)         C(23)-C(25)         1.501(2)           N(1)-C(1)         1.332(3)         O(7)-C(28)         1.202(7)           N(1)-C(5)         1.339(3)         N(3)-C(26)         1.442(7)           N(2)-C(6)         1.476(3)         N(3)-C(28)         1.341(6)           N(2)-C(7)         1.394(4)         N(3)-C(28)         1.341(6)           N(2)-C(7)         1.394(4)         N(3)-C(28)         1.341(6)           N(2)-C(8)         1.387(3)         O(8)-C(31)         1.248(9)           C(1)-C(2)         1.373(4)         N(4)-C(30)         1.351(8)           C(3)-C(4)         1.366(4)         N(4)-C(31)         1.367(6)           C(4)-C(5)         1.383(3)         O(9)-C(33)         1.426(7)           C(4)-C(6)         1.506(4)         N(5)-C(34)         1.426(8)	O(3)-C(14)	1.256(3)	C(18)-C(24)	1.415(3)
O(4)-C(14)         1.250(3)         C(19)-C(21)         1.419(3)           O(5)-Zn(1)#4         2.0435(14)         C(21)-C(22)         1.361(3)           O(5)-C(25)         1.258(3)         C(22)-C(23)         1.412(3)           O(6)-Zn(1)#5         2.0441(14)         C(23)-C(24)         1.370(3)           O(6)-C(25)         1.251(3)         C(23)-C(25)         1.501(2)           N(1)-C(1)         1.332(3)         O(7)-C(28)         1.202(7)           N(1)-C(5)         1.339(3)         N(3)-C(26)         1.442(7)           N(2)-C(6)         1.476(3)         N(3)-C(28)         1.341(6)           N(2)-C(7)         1.394(4)         N(3)-C(28)         1.341(6)           N(2)-C(7)         1.394(4)         N(4)-C(29)         1.430(7)           C(1)-C(2)         1.373(4)         N(4)-C(29)         1.430(7)           C(2)-C(3)         1.379(5)         N(4)-C(30)         1.351(8)           C(3)-C(4)         1.366(4)         N(4)-C(31)         1.367(6)           C(4)-C(5)         1.383(3)         O(9)-C(33)         1.192(7)           C(4)-C(6)         1.506(4)         N(5)-C(32)         1.468(8)           C(7)-C(11)         1.484(4)         N(5)-C(33)         1.426(7)      C	O(4)-Zn(1)#1	2.0453(14)	C(19)-C(20)	1.416(3)
O(5)-Zn(1)#4         2.0435(14)         C(21)-C(22)         1.361(3)           O(5)-C(25)         1.258(3)         C(22)-C(23)         1.412(3)           O(6)-C(25)         1.251(3)         C(23)-C(24)         1.370(3)           O(6)-C(25)         1.251(3)         C(23)-C(25)         1.501(2)           N(1)-C(1)         1.332(3)         O(7)-C(28)         1.202(7)           N(1)-C(5)         1.339(3)         N(3)-C(26)         1.442(7)           N(2)-C(6)         1.476(3)         N(3)-C(27)         1.375(5)           N(2)-C(7)         1.394(4)         N(3)-C(28)         1.341(6)           N(2)-C(7)         1.394(4)         N(3)-C(28)         1.341(6)           N(2)-C(7)         1.394(4)         N(3)-C(28)         1.341(6)           N(2)-C(7)         1.394(4)         N(4)-C(29)         1.430(7)           C(1)-C(2)         1.373(4)         N(4)-C(30)         1.351(8)           C(3)-C(4)         1.366(4)         N(4)-C(31)         1.367(6)           C(4)-C(5)         1.383(3)         O(9)-C(33)         1.426(7)           C(4)-C(6)         1.506(4)         N(5)-C(32)         1.468(8)           C(7)-C(11)         1.480(4)         N(5A)-C(33A)         1.215(8)	O(4)-C(14)	1.250(3)	C(19)-C(21)	1.419(3)
O(5)-C(25)         1.258(3)         C(22)-C(23)         1.412(3)           O(6)-Zn(1)#5         2.0441(14)         C(23)-C(24)         1.370(3)           O(6)-C(25)         1.251(3)         C(23)-C(25)         1.501(2)           N(1)-C(1)         1.332(3)         O(7)-C(28)         1.202(7)           N(1)-C(5)         1.339(3)         N(3)-C(26)         1.442(7)           N(2)-C(6)         1.476(3)         N(3)-C(28)         1.341(6)           N(2)-C(7)         1.394(4)         N(3)-C(28)         1.341(6)           N(2)-C(7)         1.394(4)         N(3)-C(28)         1.341(6)           N(2)-C(8)         1.387(3)         O(8)-C(31)         1.248(9)           C(1)-C(2)         1.373(4)         N(4)-C(29)         1.430(7)           C(2)-C(3)         1.379(5)         N(4)-C(30)         1.351(8)           C(3)-C(4)         1.366(4)         N(4)-C(31)         1.367(6)           C(4)-C(5)         1.383(3)         O(9)-C(33)         1.192(7)           C(4)-C(6)         1.506(4)         N(5)-C(32)         1.468(8)           C(7)-C(11)         1.484(4)         N(5)-C(33)         1.422(7)           C(8)-C(9)         1.406(4)         O(9A)-C(33A)         1.215(8)	O(5)-Zn(1)#4	2.0435(14)	C(21)-C(22)	1.361(3)
O(6)-Zn(1)#5         2.0441(14)         C(23)-C(24)         1.370(3)           O(6)-C(25)         1.251(3)         C(23)-C(25)         1.501(2)           N(1)-C(1)         1.332(3)         O(7)-C(28)         1.202(7)           N(1)-C(5)         1.339(3)         N(3)-C(26)         1.442(7)           N(2)-C(6)         1.476(3)         N(3)-C(27)         1.375(5)           N(2)-C(7)         1.394(4)         N(3)-C(28)         1.341(6)           N(2)-C(8)         1.387(3)         O(8)-C(31)         1.248(9)           C(1)-C(2)         1.373(4)         N(4)-C(29)         1.430(7)           C(2)-C(3)         1.379(5)         N(4)-C(30)         1.351(8)           C(3)-C(4)         1.366(4)         N(4)-C(31)         1.367(6)           C(4)-C(5)         1.383(3)         O(9)-C(33)         1.192(7)           C(4)-C(6)         1.506(4)         N(5)-C(32)         1.468(8)           C(7)-C(11)         1.484(4)         N(5)-C(33)         1.426(7)           C(8)-C(9)         1.480(4)         N(5A)-C(32A)         1.476(8)           C(10)-C(10)         1.406(4)         O(9A)-C(33A)         1.215(8)           C(9)-C(13)         1.374(4)         N(5A)-C(32A)         1.476(8)	O(5)-C(25)	1.258(3)	C(22)-C(23)	1.412(3)
O(6)-C(25)         1.251(3)         C(23)-C(25)         1.501(2)           N(1)-C(1)         1.332(3)         O(7)-C(28)         1.202(7)           N(1)-C(5)         1.339(3)         N(3)-C(26)         1.442(7)           N(2)-C(6)         1.476(3)         N(3)-C(28)         1.341(6)           N(2)-C(7)         1.394(4)         N(3)-C(28)         1.341(6)           N(2)-C(8)         1.387(3)         O(8)-C(31)         1.248(9)           C(1)-C(2)         1.373(4)         N(4)-C(29)         1.430(7)           C(2)-C(3)         1.379(5)         N(4)-C(30)         1.351(8)           C(3)-C(4)         1.366(4)         N(4)-C(31)         1.367(6)           C(4)-C(5)         1.383(3)         O(9)-C(33)         1.192(7)           C(4)-C(6)         1.506(4)         N(5)-C(32)         1.468(8)           C(7)-C(11)         1.484(4)         N(5)-C(33)         1.426(7)           C(8)-C(9)         1.480(4)         N(5)-C(33A)         1.215(8)           C(9)-C(10)         1.406(4)         O(9A)-C(33A)         1.215(8)           C(10)-C(10)#6         1.416(5)         N(5A)-C(3AA)         1.427(8)           C(10)-C(10)#6         1.416(5)         N(5A)-C(3AA)         1.447(8)      C	O(6)-Zn(1)#5	2.0441(14)	C(23)-C(24)	1.370(3)
N(1)-C(1)         1.332(3)         O(7)-C(28)         1.202(7)           N(1)-C(5)         1.339(3)         N(3)-C(26)         1.442(7)           N(2)-C(6)         1.476(3)         N(3)-C(27)         1.375(5)           N(2)-C(7)         1.394(4)         N(3)-C(28)         1.341(6)           N(2)-C(8)         1.387(3)         O(8)-C(31)         1.248(9)           C(1)-C(2)         1.373(4)         N(4)-C(29)         1.430(7)           C(2)-C(3)         1.379(5)         N(4)-C(30)         1.351(8)           C(3)-C(4)         1.366(4)         N(4)-C(31)         1.367(6)           C(4)-C(5)         1.383(3)         O(9)-C(33)         1.192(7)           C(4)-C(6)         1.506(4)         N(5)-C(32)         1.468(8)           C(7)-C(11)         1.484(4)         N(5)-C(33)         1.426(7)           C(8)-C(9)         1.480(4)         N(5)-C(33A)         1.215(8)           C(9)-C(10)         1.406(4)         O(9A)-C(33A)         1.215(8)           C(9)-C(13)         1.374(4)         N(5A)-C(32A)         1.447(8)           C(10)-C(10)#6         1.416(5)         N(5A)-C(33A)         1.421(8)           C(10)-C(10)#6         1.416(5)         N(5A)-C(34A)         1.447(8)	O(6)-C(25)	1.251(3)	C(23)-C(25)	1.501(2)
N(1)-C(5)       1.339(3)       N(3)-C(26)       1.442(7)         N(2)-C(6)       1.476(3)       N(3)-C(27)       1.375(5)         N(2)-C(7)       1.394(4)       N(3)-C(28)       1.341(6)         N(2)-C(8)       1.387(3)       O(8)-C(31)       1.248(9)         C(1)-C(2)       1.373(4)       N(4)-C(29)       1.430(7)         C(2)-C(3)       1.379(5)       N(4)-C(30)       1.351(8)         C(3)-C(4)       1.366(4)       N(4)-C(31)       1.367(6)         C(4)-C(5)       1.383(3)       O(9)-C(33)       1.192(7)         C(4)-C(6)       1.506(4)       N(5)-C(32)       1.468(8)         C(7)-C(11)       1.484(4)       N(5)-C(33)       1.426(7)         C(8)-C(9)       1.480(4)       N(5)-C(34)       1.427(8)         C(9)-C(10)       1.406(4)       O(9A)-C(33A)       1.215(8)         C(10)-C(10)#6       1.416(5)       N(5A)-C(33A)       1.421(8)         C(10)-C(11)       1.405(4)       N(5A)-C(33A)       1.421(8)         C(10)-C(11)       1.405(4)       N(5A)-C(34A)       1.447(8)         C(11)-C(12)       1.370(4)	N(1)-C(1)	1.332(3)	O(7)-C(28)	1.202(7)
N(2)-C(6)       1.476(3)       N(3)-C(27)       1.375(5)         N(2)-C(7)       1.394(4)       N(3)-C(28)       1.341(6)         N(2)-C(8)       1.387(3)       O(8)-C(31)       1.248(9)         C(1)-C(2)       1.373(4)       N(4)-C(29)       1.430(7)         C(2)-C(3)       1.379(5)       N(4)-C(30)       1.351(8)         C(3)-C(4)       1.366(4)       N(4)-C(31)       1.367(6)         C(4)-C(5)       1.383(3)       O(9)-C(33)       1.192(7)         C(4)-C(6)       1.506(4)       N(5)-C(32)       1.468(8)         C(7)-C(11)       1.484(4)       N(5)-C(33)       1.426(7)         C(8)-C(9)       1.480(4)       N(5)-C(34)       1.427(8)         C(9)-C(10)       1.406(4)       O(9A)-C(33A)       1.215(8)         C(9)-C(10)       1.406(4)       O(9A)-C(33A)       1.215(8)         C(10)-C(10)#6       1.416(5)       N(5A)-C(32A)       1.447(8)         C(10)-C(11)       1.405(4)       N(5A)-C(33A)       1.421(8)         C(10)-C(11)       1.405(4)       N(5A)-C(34A)       1.447(8)         C(11)-C(12)       1.370(4)       1.447(8)       C(11)-C(7)       119.4(3)         O(3)-Zn(1)-O(4)#1       159.04(7)       C(12)-C(11)-C(7)	N(1)-C(5)	1.339(3)	N(3)-C(26)	1.442(7)
N(2)-C(7)       1.394(4)       N(3)-C(28)       1.341(6)         N(2)-C(8)       1.387(3)       O(8)-C(31)       1.248(9)         C(1)-C(2)       1.373(4)       N(4)-C(29)       1.430(7)         C(2)-C(3)       1.379(5)       N(4)-C(30)       1.351(8)         C(3)-C(4)       1.366(4)       N(4)-C(31)       1.367(6)         C(4)-C(5)       1.383(3)       O(9)-C(33)       1.192(7)         C(4)-C(6)       1.506(4)       N(5)-C(32)       1.468(8)         C(7)-C(11)       1.484(4)       N(5)-C(33)       1.426(7)         C(8)-C(9)       1.480(4)       N(5)-C(34)       1.427(8)         C(9)-C(10)       1.406(4)       O(9A)-C(33A)       1.215(8)         C(9)-C(10)       1.405(4)       N(5A)-C(32A)       1.476(8)         C(10)-C(10)#6       1.416(5)       N(5A)-C(33A)       1.421(8)         C(10)-C(11)       1.405(4)       N(5A)-C(34A)       1.447(8)         C(11)-C(12)       1.370(4)       .       .         V       V       V       V       V         O(3)-Zn(1)-O(4)#1       159.04(7)       C(12)-C(11)-C(7)       119.4(3)         O(3)-Zn(1)-O(5)#2       87.54(7)       C(12)-C(11)-C(7)       120.2(3)	N(2)-C(6)	1.476(3)	N(3)-C(27)	1.375(5)
N(2)-C(8)1.387(3) $O(8)$ -C(31)1.248(9)C(1)-C(2)1.373(4)N(4)-C(29)1.430(7)C(2)-C(3)1.379(5)N(4)-C(30)1.351(8)C(3)-C(4)1.366(4)N(4)-C(31)1.367(6)C(4)-C(5)1.383(3) $O(9)$ -C(33)1.192(7)C(4)-C(6)1.506(4)N(5)-C(32)1.468(8)C(7)-C(11)1.484(4)N(5)-C(33)1.426(7)C(8)-C(9)1.480(4)N(5)-C(34)1.427(8)C(9)-C(10)1.406(4) $O(9A)$ -C(33A)1.215(8)C(9)-C(13)1.374(4)N(5A)-C(32A)1.476(8)C(10)-C(10)#61.416(5)N(5A)-C(33A)1.421(8)C(10)-C(11)1.405(4)N(5A)-C(34A)1.447(8)C(11)-C(12)1.370(4)VVVVVVO(3)-Zn(1)-O(4)#1159.04(7)C(12)-C(11)-C(7)119.4(3)O(3)-Zn(1)-O(5)#287.54(7)C(12)-C(11)-C(10)120.4(3)O(3)-Zn(1)-O(6)#389.48(8)C(11)-C(12)-C(13)#6120.5(3)	N(2)-C(7)	1.394(4)	N(3)-C(28)	1.341(6)
C(1)-C(2)1.373(4)N(4)-C(29)1.430(7) $C(2)-C(3)$ 1.379(5)N(4)-C(30)1.351(8) $C(3)-C(4)$ 1.366(4)N(4)-C(31)1.367(6) $C(4)-C(5)$ 1.383(3) $O(9)-C(33)$ 1.192(7) $C(4)-C(6)$ 1.506(4)N(5)-C(32)1.468(8) $C(7)-C(11)$ 1.484(4)N(5)-C(33)1.426(7) $C(8)-C(9)$ 1.480(4)N(5)-C(34)1.427(8) $C(9)-C(10)$ 1.406(4) $O(9A)-C(33A)$ 1.215(8) $C(9)-C(13)$ 1.374(4)N(5A)-C(32A)1.476(8) $C(10)-C(10)$ #61.416(5)N(5A)-C(33A)1.421(8) $C(10)-C(11)$ 1.405(4)N(5A)-C(34A)1.447(8) $C(11)-C(12)$ 1.370(4)1.447(8) $C(3)-Zn(1)-Zn(1)$ #184.82(5) $C(10)-C(11)-C(7)$ 119.4(3) $O(3)-Zn(1)-O(4)$ #1159.04(7) $C(12)-C(11)-C(7)$ 120.2(3) $O(3)-Zn(1)-O(5)$ #287.54(7) $C(12)-C(11)-C(10)$ 120.4(3) $O(3)-Zn(1)-O(6)$ #389.48(8) $C(11)-C(12)-C(13)$ #6120.5(3)	N(2)-C(8)	1.387(3)	O(8)-C(31)	1.248(9)
C(2)-C(3)1.379(5)N(4)-C(30)1.351(8) $C(3)-C(4)$ 1.366(4)N(4)-C(31)1.367(6) $C(4)-C(5)$ 1.383(3)O(9)-C(33)1.192(7) $C(4)-C(6)$ 1.506(4)N(5)-C(32)1.468(8) $C(7)-C(11)$ 1.484(4)N(5)-C(33)1.426(7) $C(8)-C(9)$ 1.480(4)N(5)-C(34)1.427(8) $C(9)-C(10)$ 1.406(4)O(9A)-C(33A)1.215(8) $C(9)-C(10)$ 1.406(4)N(5A)-C(32A)1.476(8) $C(10)-C(10)$ #61.416(5)N(5A)-C(33A)1.421(8) $C(10)-C(11)$ 1.405(4)N(5A)-C(34A)1.447(8) $C(10)-C(11)$ 1.370(4)N(5A)-C(34A)1.447(8) $C(11)-C(12)$ 1.370(4) $V(5A)-C(34A)$ 1.447(8) $C(3)-Zn(1)-O(4)$ #1159.04(7) $C(12)-C(11)-C(7)$ 119.4(3) $O(3)-Zn(1)-O(5)$ #287.54(7) $C(12)-C(11)-C(10)$ 120.4(3) $O(3)-Zn(1)-O(6)$ #389.48(8) $C(11)-C(12)-C(13)$ #6120.5(3)	C(1)-C(2)	1.373(4)	N(4)-C(29)	1.430(7)
C(3)-C(4)1.366(4)N(4)-C(31)1.367(6)C(4)-C(5)1.383(3)O(9)-C(33)1.192(7)C(4)-C(6)1.506(4)N(5)-C(32)1.468(8)C(7)-C(11)1.484(4)N(5)-C(33)1.426(7)C(8)-C(9)1.480(4)N(5)-C(34)1.427(8)C(9)-C(10)1.406(4)O(9A)-C(33A)1.215(8)C(9)-C(13)1.374(4)N(5A)-C(32A)1.476(8)C(10)-C(10)#61.416(5)N(5A)-C(33A)1.421(8)C(10)-C(11)1.405(4)N(5A)-C(34A)1.447(8)C(11)-C(12)1.370(4)N1.447(8)O(3)-Zn(1)-O(4)#1159.04(7)C(12)-C(11)-C(7)119.4(3)O(3)-Zn(1)-O(5)#287.54(7)C(12)-C(11)-C(10)120.4(3)O(3)-Zn(1)-O(6)#389.48(8)C(11)-C(12)-C(13)#6120.5(3)	C(2)-C(3)	1.379(5)	N(4)-C(30)	1.351(8)
C(4)-C(5)1.383(3) $O(9)-C(33)$ 1.192(7) $C(4)-C(6)$ 1.506(4) $N(5)-C(32)$ 1.468(8) $C(7)-C(11)$ 1.484(4) $N(5)-C(33)$ 1.426(7) $C(8)-C(9)$ 1.480(4) $N(5)-C(34)$ 1.427(8) $C(9)-C(10)$ 1.406(4) $O(9A)-C(33A)$ 1.215(8) $C(9)-C(13)$ 1.374(4) $N(5A)-C(32A)$ 1.476(8) $C(10)-C(10)$ #61.416(5) $N(5A)-C(33A)$ 1.421(8) $C(10)-C(11)$ 1.405(4) $N(5A)-C(34A)$ 1.447(8) $C(11)-C(12)$ 1.370(4) $V(5A)-C(34A)$ 1.447(8) $O(3)-Zn(1)-Zn(1)$ #184.82(5) $C(10)-C(11)-C(7)$ 119.4(3) $O(3)-Zn(1)-O(4)$ #1159.04(7) $C(12)-C(11)-C(7)$ 120.2(3) $O(3)-Zn(1)-O(5)$ #287.54(7) $C(12)-C(11)-C(10)$ 120.4(3) $O(3)-Zn(1)-O(6)$ #389.48(8) $C(11)-C(12)-C(13)$ #6120.5(3)	C(3)-C(4)	1.366(4)	N(4)-C(31)	1.367(6)
C(4)-C(6)1.506(4)N(5)-C(32)1.468(8) $C(7)-C(11)$ 1.484(4)N(5)-C(33)1.426(7) $C(8)-C(9)$ 1.480(4)N(5)-C(34)1.427(8) $C(9)-C(10)$ 1.406(4) $O(9A)-C(33A)$ 1.215(8) $C(9)-C(13)$ 1.374(4)N(5A)-C(32A)1.476(8) $C(10)-C(10)#6$ 1.416(5)N(5A)-C(33A)1.421(8) $C(10)-C(11)$ 1.405(4)N(5A)-C(33A)1.421(8) $C(11)-C(12)$ 1.370(4)N(5A)-C(34A)1.447(8) $O(3)-Zn(1)-O(4)#1$ 159.04(7) $C(12)-C(11)-C(7)$ 119.4(3) $O(3)-Zn(1)-O(5)#2$ 87.54(7) $C(12)-C(11)-C(70)$ 120.2(3) $O(3)-Zn(1)-O(6)#3$ 89.48(8) $C(11)-C(12)-C(13)#6$ 120.5(3)	C(4)-C(5)	1.383(3)	O(9)-C(33)	1.192(7)
$\begin{array}{cccccc} C(7)-C(11) & 1.484(4) & N(5)-C(33) & 1.426(7) \\ C(8)-C(9) & 1.480(4) & N(5)-C(34) & 1.427(8) \\ C(9)-C(10) & 1.406(4) & O(9A)-C(33A) & 1.215(8) \\ C(9)-C(13) & 1.374(4) & N(5A)-C(32A) & 1.476(8) \\ C(10)-C(10)#6 & 1.416(5) & N(5A)-C(33A) & 1.421(8) \\ C(10)-C(11) & 1.405(4) & N(5A)-C(34A) & 1.447(8) \\ C(11)-C(12) & 1.370(4) & & & & & & \\ \end{array}$	C(4)-C(6)	1.506(4)	N(5)-C(32)	1.468(8)
C(8)-C(9)1.480(4)N(5)-C(34)1.427(8) $C(9)-C(10)$ 1.406(4) $O(9A)-C(33A)$ 1.215(8) $C(9)-C(13)$ 1.374(4) $N(5A)-C(32A)$ 1.476(8) $C(10)-C(10)#6$ 1.416(5) $N(5A)-C(33A)$ 1.421(8) $C(10)-C(11)$ 1.405(4) $N(5A)-C(34A)$ 1.447(8) $C(11)-C(12)$ 1.370(4) $V(5A)-C(34A)$ 1.447(8) $O(3)-Zn(1)-Zn(1)#1$ 84.82(5) $C(10)-C(11)-C(7)$ 119.4(3) $O(3)-Zn(1)-O(4)#1$ 159.04(7) $C(12)-C(11)-C(7)$ 120.2(3) $O(3)-Zn(1)-O(5)#2$ 87.54(7) $C(12)-C(11)-C(10)$ 120.4(3) $O(3)-Zn(1)-O(6)#3$ 89.48(8) $C(11)-C(12)-C(13)#6$ 120.5(3)	C(7)-C(11)	1.484(4)	N(5)-C(33)	1.426(7)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(8)-C(9)	1.480(4)	N(5)-C(34)	1.427(8)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(9)-C(10)	1.406(4)	O(9A)-C(33A)	1.215(8)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(9)-C(13)	1.374(4)	N(5A)-C(32A)	1.476(8)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(10)-C(10)#6	1.416(5)	N(5A)-C(33A)	1.421(8)
C(11)-C(12) $1.370(4)$ $O(3)-Zn(1)-Zn(1)#1$ $84.82(5)$ $C(10)-C(11)-C(7)$ $119.4(3)$ $O(3)-Zn(1)-O(4)#1$ $159.04(7)$ $C(12)-C(11)-C(7)$ $120.2(3)$ $O(3)-Zn(1)-O(5)#2$ $87.54(7)$ $C(12)-C(11)-C(10)$ $120.4(3)$ $O(3)-Zn(1)-O(6)#3$ $89.48(8)$ $C(11)-C(12)-C(13)#6$ $120.5(3)$	C(10)-C(11)	1.405(4)	N(5A)-C(34A)	1.447(8)
O(3)-Zn(1)-Zn(1)#184.82(5)C(10)-C(11)-C(7)119.4(3)O(3)-Zn(1)-O(4)#1159.04(7)C(12)-C(11)-C(7)120.2(3)O(3)-Zn(1)-O(5)#287.54(7)C(12)-C(11)-C(10)120.4(3)O(3)-Zn(1)-O(6)#389.48(8)C(11)-C(12)-C(13)#6120.5(3)O(2) Z_1(1) V(1)120.2(2)20(2) Z_1(12) V(12) V(	C(11)-C(12)	1.370(4)		
O(3)-Zn(1)-O(4)#1       159.04(7)       C(12)-C(11)-C(7)       120.2(3)         O(3)-Zn(1)-O(5)#2       87.54(7)       C(12)-C(11)-C(10)       120.4(3)         O(3)-Zn(1)-O(6)#3       89.48(8)       C(11)-C(12)-C(13)#6       120.5(3)         O(2) Z_1(1) V(1)       120.2(Z)       20(Z) Z(12) V(12) Z(12) V(12) V(12	O(3)-Zn(1)-Zn(1)#1	84.82(5)	C(10)-C(11)-C(7)	119.4(3)
O(3)-Zn(1)-O(5)#2       87.54(7)       C(12)-C(11)-C(10)       120.4(3)         O(3)-Zn(1)-O(6)#3       89.48(8)       C(11)-C(12)-C(13)#6       120.5(3)         O(2) Z_1(1) V(1)       122.62(Z)       2(2) Z(12) V(12)	O(3)-Zn(1)-O(4)#1	159.04(7)	C(12)-C(11)-C(7)	120.2(3)
O(3)-Zn(1)-O(6)#3 89.48(8) C(11)-C(12)-C(13)#6 120.5(3)	O(3)-Zn(1)-O(5)#2	87.54(7)	C(12)-C(11)-C(10)	120.4(3)
	O(3)-Zn(1)-O(6)#3	89.48(8)	C(11)-C(12)-C(13)#6	120.5(3)
U(3)-Zn(1)-N(1) 103.63(7) C(9)-C(13)-C(12)#6 120.4(3)	O(3)-Zn(1)-N(1)	103.63(7)	C(9)-C(13)-C(12)#6	120.4(3)

Table S2. Selected bond lengths (Å) and angles (°) for 1@DMF.

O(4)#1 <sup>-</sup> Zn(1)-Zn(1)#1	74.22(5)	O(3)-C(14)-C(15)	117.13(19)
O(5)#2 <sup>-</sup> Zn(1)-Zn(1)#1	79.39(5)	O(4)-C(14)-O(3)	125.70(18)
O(5)#2 <sup>-</sup> Zn(1)-O(4)#1	88.47(8)	O(4)-C(14)-C(15)	117.17(18)
O(5)#2 <sup>-</sup> Zn(1)-O(6)#3	159.25(7)	C(16)-C(15)-C(14)	120.28(19)
O(6)#3 <sup>-</sup> Zn(1)-Zn(1)#1	79.90(5)	C(20)-C(15)-C(14)	119.79(19)
O(6)#3 <sup>-</sup> Zn(1)-O(4)#1	87.01(7)	C(20)-C(15)-C(16)	119.92(18)
N(1)-Zn(1)-Zn(1)#1	171.52(6)	C(17)-C(16)-C(15)	120.8(2)
N(1)-Zn(1)-O(4)#1	97.33(7)	C(16)-C(17)-C(18)	120.5(2)
N(1)-Zn(1)-O(5)#2	101.46(7)	C(19)-C(18)-C(17)	118.93(18)
N(1)-Zn(1)-O(6)#3	99.20(7)	C(19)-C(18)-C(24)	118.90(19)
C(14)-O(3)-Zn(1)	120.84(14)	C(24)-C(18)-C(17)	122.17(19)
C(14)-O(4)-Zn(1)#1	134.39(14)	C(18)-C(19)-C(20)	119.06(19)
C(25)-O(5)-Zn(1)#4	127.55(13)	C(18)-C(19)-C(21)	118.79(19)
C(25)-O(6)-Zn(1)#5	126.88(14)	C(20)-C(19)-C(21)	122.2(2)
C(10)-C(9)-C(8)	119.8(2)	C(34)-N(5)-C(32)	118.4(7)
C(13)-C(9)-C(8)	120.1(3)	O(9)-C(33)-N(5)	122.1(10)
C(13)-C(9)-C(10)	120.1(3)	C(33A)-N(5A)-C(32A)	108.1(9)
C(9)-C(10)-C(10)#6	119.4(3)	C(33A)-N(5A)-C(34A)	138.5(12)

<sup>1</sup>2-X,1-Y,1-Z; <sup>2</sup>+X,1/2-Y,-1/2+Z; <sup>3</sup>2-X,1/2+Y,3/2-Z; <sup>4</sup>+X,1/2-Y,1/2+Z; <sup>5</sup>2-X,-1/2+Y,3/2-Z; <sup>6</sup>1-X,1-Y,-Z

	Comp	ound 1@DMF		
D-H…A	d(D-H)	d(H…A)	d(D…A)	<(DH/
C(1)-H(1) O(6)	0.930	2.580	3.164	121.2
C(5)-H(5) O(2)	0.930	2.605	3.276	129.4
C(26)-H(26A) O(1)	0.960	2.605	3.258	125.4
C(29)-H(29A) O(7)	0.960	2.474	3.432	175.5
C(32)-H(32C) O(8)	0.960	2.620	3.396	138.0

Table S3. Hydrogen bonds of for 1@DMF (Å and °).