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# Photochromism and photoresponsive luminescence in naphthalenediimide coordination polymers with high thermostability

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**Table S1a** Selected bond length and angles of compound **1**.

| | | | |
|---|---|---|---|
| Zn2—O8 | 1.9359(13) | Zn1—N8$^{\#2}$ | 2.0411 (16) |
| Zn2—O1$^{\#1}$ | 1.9659 (14) | Zn1—N7$^{\#2}$ | 2.0528 (16) |
| Zn2—N1 | 2.0358 (16) | O1—Zn2$^{\#3}$ | 1.9659 (14) |
| Zn2—N2 | 2.0387 (16) | N8—Zn1$^{\#4}$ | 2.0411 (16) |
| Zn1—O5 | 1.9556 (14) | N7—Zn1$^{\#4}$ | 2.0528 (16) |
| Zn1—O4 | 1.9544 (14) | | |
| O8—Zn2—N1 | 116.24 (6) | C15—O5—Zn1 | 109.74 (13) |
| O8—Zn2—N2 | 108.72 (6) | C14—O4—Zn1 | 125.27 (14) |
| O1$^{\#1}$—Zn2—N1 | 102.62 (6) | C1—O1—Zn2$^{\#3}$ | 123.70 (15) |
| O1$^{\#1}$—Zn2—N2 | 110.84 (6) | C49—N8—Zn1$^{\#4}$ | 114.27 (17) |
| N1—Zn2—N2 | 114.06 (6) | C50—N8—Zn1$^{\#4}$ | 127.36 (13) |
| O5—Zn1—N8$^{\#2}$ | 121.52 (6) | C57—N1—Zn2 | 117.50 (13) |
| O5—Zn1—N7$^{\#2}$ | 111.81 (6) | C53—N1—Zn2 | 123.80 (13) |
| O4—Zn1—O5 | 98.62 (6) | C72—N7—Zn1$^{\#4}$ | 122.23 (12) |
| O4—Zn1—N8$^{\#2}$ | 102.86 (6) | C76—N7—Zn1$^{\#4}$ | 119.48 (13) |
| O4—Zn1—N7$^{\#2}$ | 114.98 (6) | C29—N2—Zn2 | 121.08 (13) |
| N8$^{\#2}$—Zn1—N7$^{\#2}$ | 106.84 (6) | C33—N2—Zn2 | 120.20 (13) |
| C28—O8—Zn2 | 114.35 (12) | | |

Symmetry codes: #1 *x*+1, *y*−2, *z*; #2 *x*−1, *y*+2, *z*+1; #3 *x*−1, *y*+2, *z*; #4 *x*+1, *y*−2, *z*−1.

**Table S1b** Selected bond length and angles of compound **2**.

| | | | |
|---|---|---|---|
| Cd1—O5 | 2.3989 (14) | Cd1—N1 | 2.3214 (17) |
| Cd1—O8$^{\#1}$ | 2.4161 (14) | Cd1—N4$^{\#1}$ | 2.3231 (17) |
| Cd1—O7$^{\#1}$ | 2.4982 (15) | O7—Cd1$^{\#2}$ | 2.4981 (15) |
| Cd1—O9 | 2.3133 (15) | O8—Cd1$^{\#2}$ | 2.4161 (14) |
| Cd1—O6 | 2.4939 (15) | N4—Cd1$^{\#2}$ | 2.3231 (17) |
| O5—Cd1—O6 | 53.67 (5) | N1—Cd1—O8$^{\#1}$ | 88.43(5) |
| O5—Cd1—O7$^{\#1}$ | 140.63 (5) | N1—Cd1—N4$^{\#1}$ | 176.17 (6) |
| O5—Cd1—O8$^{\#1}$ | 87.42 (5) | N4$^{\#1}$—Cd1—O5 | 89.34 (5) |
| O6—Cd1—O7$^{\#1}$ | 165.45 (5) | N4$^{\#1}$—Cd1—O6 | 91.71(5) |
| O8$^{\#1}$—Cd1—O6 | 141.07 (5) | N4$^{\#1}$—Cd1—O7$^{\#1}$ | 91.23 (5) |
| O8$^{\#1}$—Cd1—O7$^{\#1}$ | 53.26 (5) | N4$^{\#1}$—Cd1—O8$^{\#1}$ | 88.49 (5) |
| O9—Cd1—O5 | 137.39 (5) | C38—O7—Cd1$^{\#2}$ | 90.62 (12) |
| O9—Cd1—O6 | 83.90(5) | C25—O5—Cd1 | 93.24 (12) |
| O9—Cd1—O7$^{\#1}$ | 81.61 (5) | C38—O8—Cd1$^{\#2}$ | 90.62(12) |
| O9—Cd1—O8$^{\#1}$ | 134.76 (5) | C25—O6—Cd1 | 89.1 (3) |
| O9—Cd1—N1 | 87.40 (6) | C5—N1—Cd1 | 121.57(14) |
| O9—Cd1—N4$^{\#1}$ | 96.39 (5) | C1—N1—Cd1$^{\#1}$ | 120.40(13) |
| N1—Cd1—O5 | 88.25 (5) | C21—N4—Cd1$^{\#4}$ | 116.68(13) |
| N1—Cd1—O6 | 89.25 (5) | C24—N4—Cd1$^{\#2}$ | 125.03 (13) |
| N1—Cd1—O7$^{\#1}$ | 88.75 (6) | | |

Symmetry codes: #1 −*x*+3/2, −*y*+1, *z*+1/2; #2 −*x*+3/2, −*y*+1, *z*−1/2.

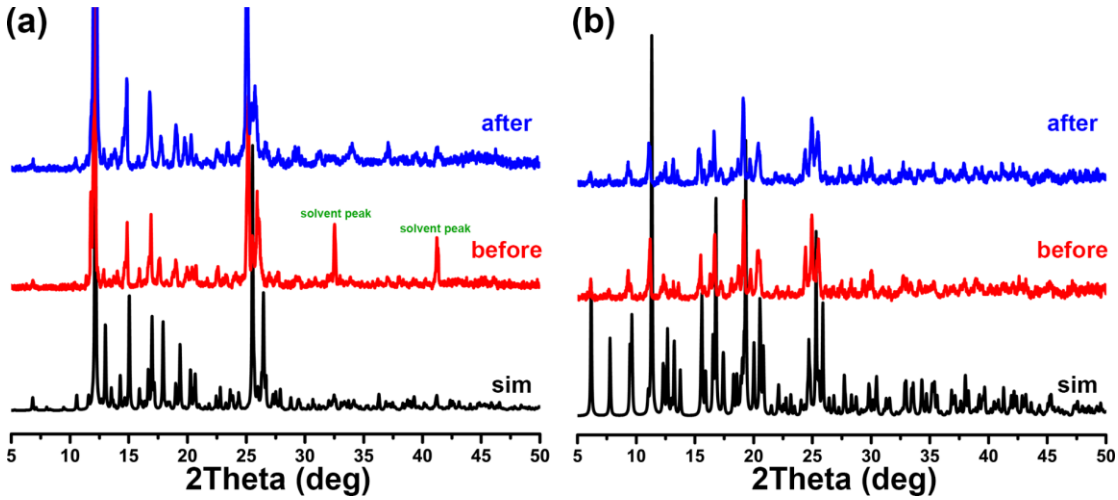


**Figure S1** PXRD patterns of compound **1** (a) and **2** (b) before and after irradiation.

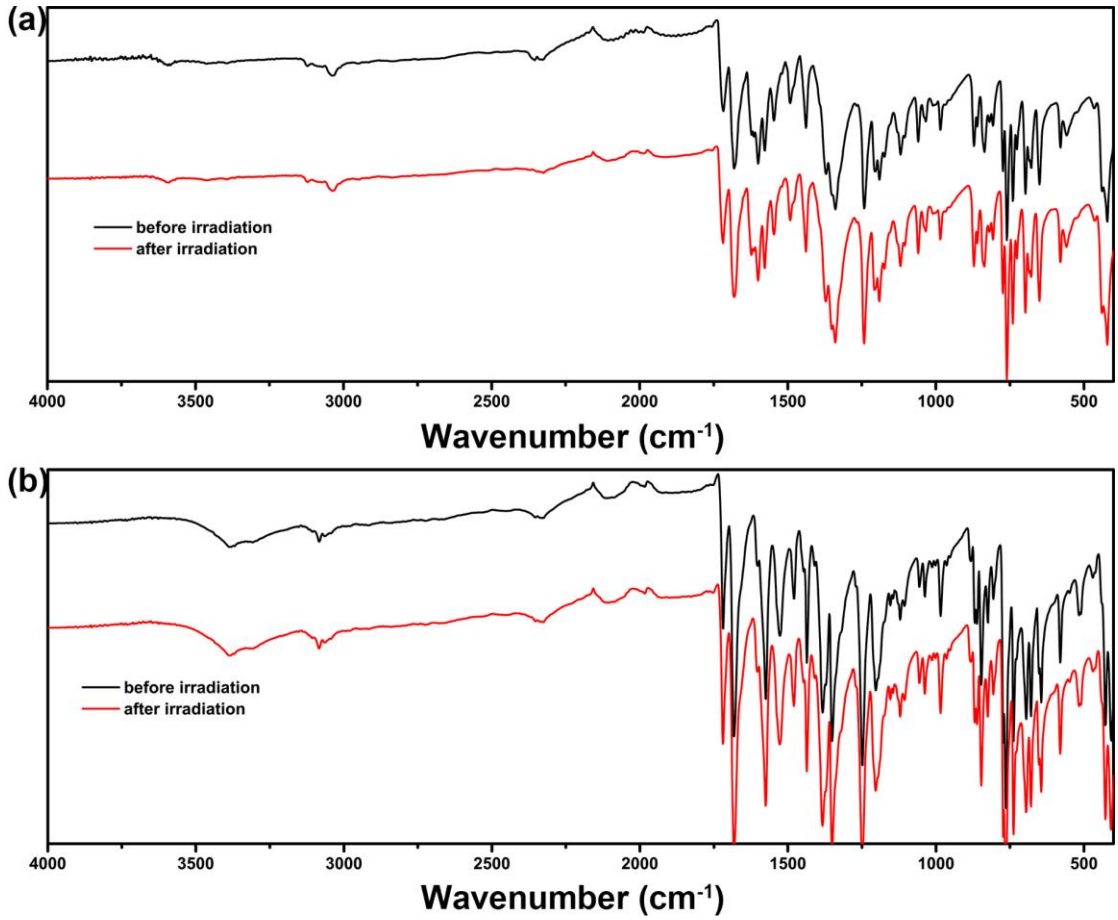


**Figure S2** FT-IR spectra of compound **1** (a) and **2** (b) before and after irradiation.

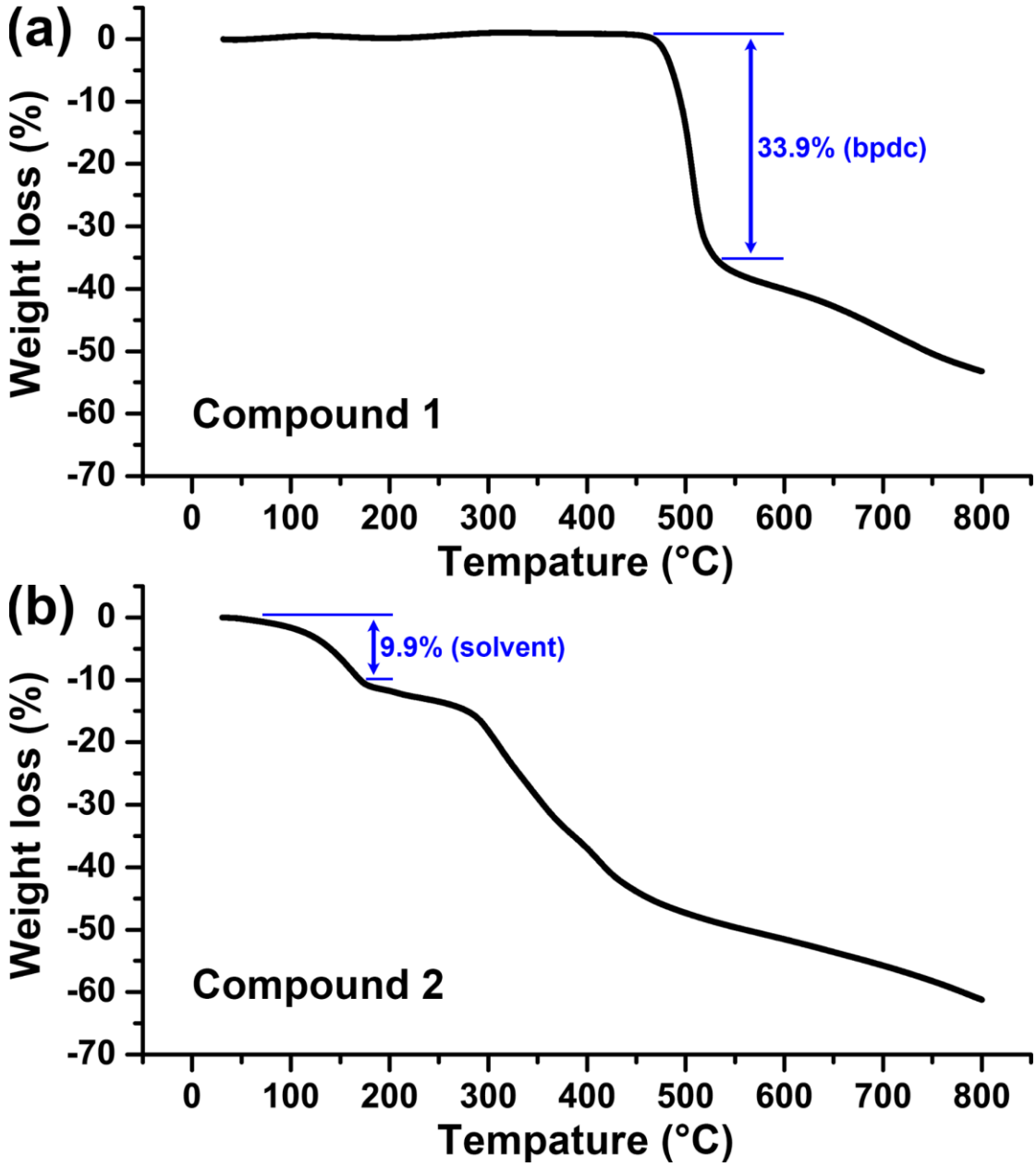


**Figure S3** TG analysis of compound **1** (a) and **2** (b).

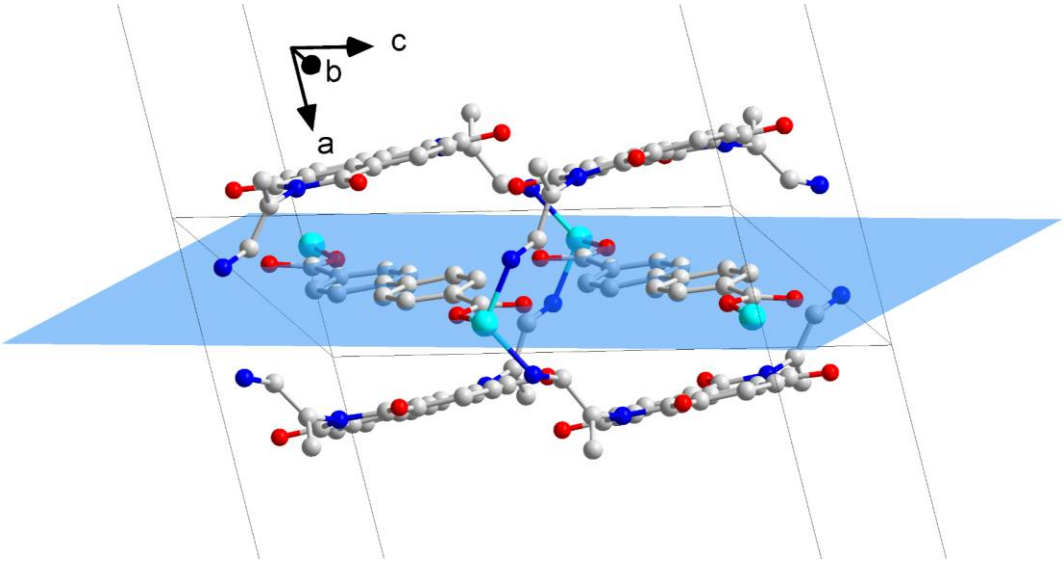


**Figure S4** (4 2 0) crystal plane in compound **1**. Legends: Zn (cyan), O (red), N (blue), C (gray).

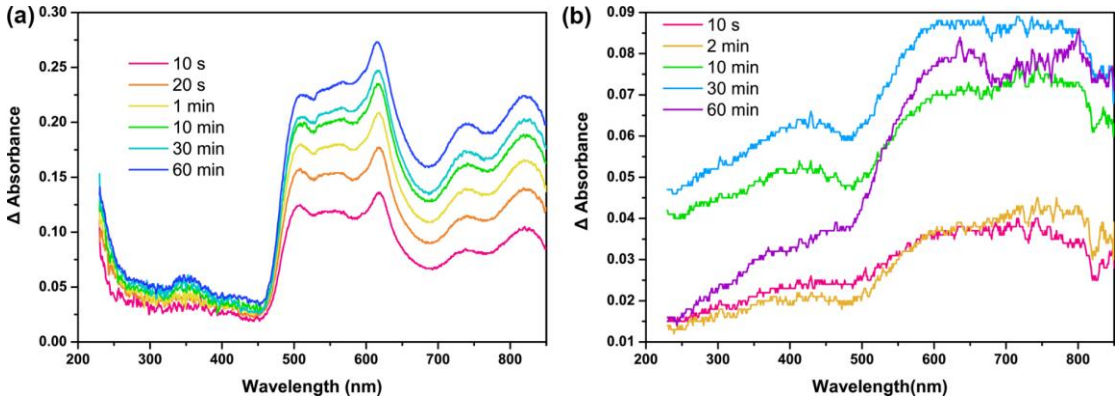


**Figure S5** Varation of time-dependent UV-vis spectra of compound **1** (a) and **2** (b).