A cadmium(II)-based metal-organic framework for selective trace
detection of nitroaniline isomers and photocatalytic degradation of
methylene blue in neutral aqueous solution

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Contents

1. X-ray Crystallography (Single-crystal diffraction) and Characterizations. S2

2. Studies on the nitro-explosives detection based on Cd–PDA. S6

3. Studies on the photodegradation of MB based on Cd–PDA. S9
1. X-ray Crystallography (Single-crystal diffraction) and Characterizations.

1.1 Figure S1 The coordination configuration of the Cd(1) and Cd(2) centre in Cd–PDA. The asymmetric mode: A: x, 1+y, z; B: 1.5-x, 0.5+y, 0.5-z.
1.2 Selective bond distance (Å) and angle (°) in Cd–PDA.

Selective bond distance (Å): Cd(1)–O(4) 2.2403(2), Cd(1)–O(8) 2.263(2), Cd(1)–O(2A) 2.3171(2), Cd(1)–O(7) 2.3192(2), Cd(1)–O(9) 2.3299(2), Cd(1)–O(1A) 2.4537(2), Cd(2)–O(12) 2.1982(2), Cd(2)–O(13B) 2.2054(2), Cd(2)–O(3) 2.2387(2), Cd(2)–O(10) 2.2864(2), Cd(2)–O(11) 2.3872(2), Cd(2)–O(20B) 2.5549(2).

Selective bond angle (°): O(4)–Cd(1)–O(8) 124.18(7), O(4)–Cd(1)–O(2A) 149.93(6), O(8)–Cd(1)–O(2A) 82.22(7), O(4)–Cd(1)–O(7) 84.03(7), O(8)–Cd(1)–O(7) 93.03(8), O(2A)–Cd(1)–O(7) 80.06(6), O(4)–Cd(1)–O(9) 94.65(7), O(8)–Cd(1)–O(9) 94.13(8), O(2A)–Cd(1)–O(9) 97.64(6), O(7)–Cd(1)–O(9) 172.11(7), O(4)–Cd(1)–O(1A) 100.41(6), O(8)–Cd(1)–O(1A) 135.41(7), O(2A)–Cd(1)–O(1A) 54.83(6), O(7)–Cd(1)–O(1A) 90.93(6), O(9)–Cd(1)–O(1A) 81.65(6), O(12)–Cd(2)–O(13B) 97.91(7), O(12)–Cd(2)–O(3) 105.45(6), O(13B)–Cd(2)–O(3) 96.67(6), O(12)–Cd(2)–O(10) 101.31(6), O(13B)–Cd(2)–O(10) 139.63(6), O(3)–Cd(2)–O(10) 111.66(6), O(12)–Cd(2)–O(11) 157.45(7), O(13B)–Cd(2)–O(11) 101.15(6), O(3)–Cd(2)–O(11) 84.24(6), O(10)–Cd(2)–O(11) 56.18(6), O(12)–Cd(2)–O(20B) 94.39(6), O(13B)–Cd(2)–O(20B) 54.45(6), O(3)–Cd(2)–O(20B) 147.42(6), O(10)–Cd(2)–O(20B) 88.77(6).
1.3 **Figure S2** PXRD patterns of the as-synthesized (red), the simulated from single X-ray crystal structure (black).

![PXRD patterns of the as-synthesized (red), the simulated from single X-ray crystal structure (black).](image)

1.4 **Figure S3** CO$_2$ adsorption/desorption isotherms of Cd–PDA at 195 K.

![CO$_2$ adsorption/desorption isotherms of Cd–PDA at 195 K.](image)
1.5 Figure S4 TGA traces of Cd-PDA ranging from room temperature to 500 °C.
2. Studies on the nitro-explosives detection based on Cd–PDA.

2.1 Figure S5 The UV/vis absorption spectra for solid Cd–PDA.

![Absorption Spectra](image)

2.2 Figure S6 The Stern–Volmer plot of Cd–PDA quenched by p-NA ethanol solution, where $I_0$ and $I$ are the fluorescence intensity before and after p-NA incorporation, respectively.

![Stern-Volmer Plot](image)

**Equation:**

$$y = 40786.8x + 0.069$$

**$R = 0.9956$**
2.3 Figure S7 Families of various fluorescence spectra of Cd–PDA in ethanol solution upon the addition of 0.125 mM of different selected analytes.
2.4 Figure S8 (Left) FT-IR spectra of o-NA (top), Cd–PDA impregnated with o-NA solution (middle) and Cd–PDA (bottom); (Right) FT-IR spectra of m-NA (top), Cd–PDA impregnated with m-NA solution (middle) and Cd–PDA (bottom).

2.5 Figure S9 Representation of the interaction between Cd–PDA and o-NA (left) and m-NA (right) computed by molecular force field-based calculations.
3. Studies on the photodegradation of MB based on Cd–PDA.

3.1 Figure S10 The first-order plots for the photodegradation of MB using Cd–PDA.

![First-order plots for photodegradation of MB using Cd–PDA](image)

3.2 Figure S11 Recycling experiments employing Cd–PDA as a catalyst for the degradation of MB under Xe lamp irradiation.

![Recycling experiments](image)