# Supporting information

## Two Anthracene Chromophores based Metal-Organic Frameworks for Gas Absorption and Promising Nitro Aromatic Sensing

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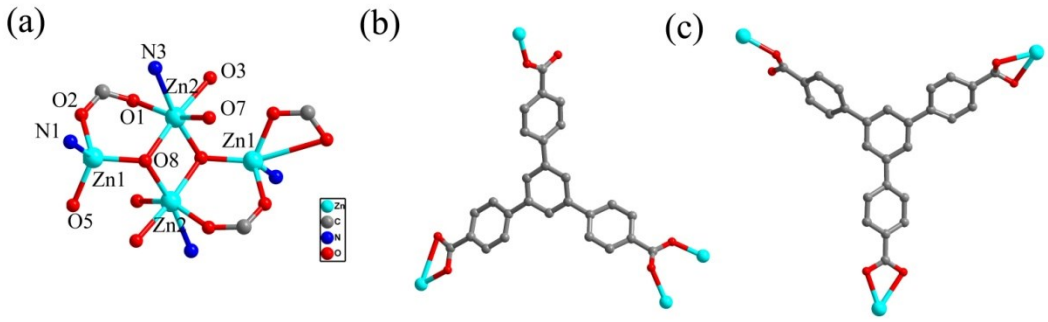


Fig. S1 (a) Tetranuclear Zn-cluster in **1**. (b) and (c) The coordination modes of btb in **1** and **2**.

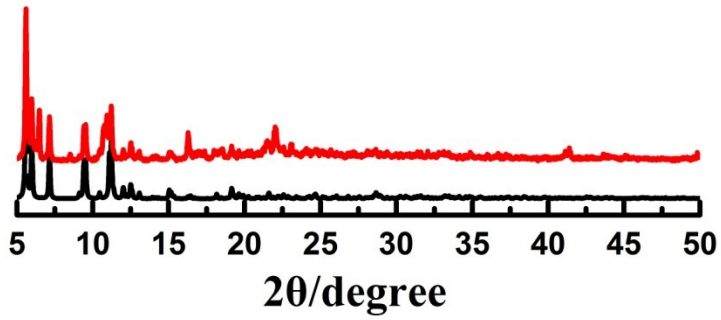


**Fig. S2** PXRD patterns for **1**.

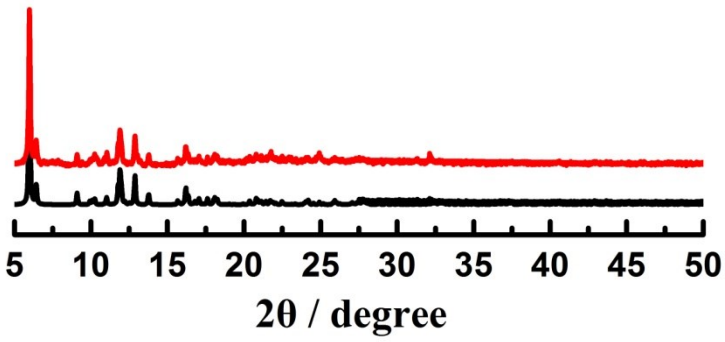


**Fig. S3** PXRD patterns for **2**.

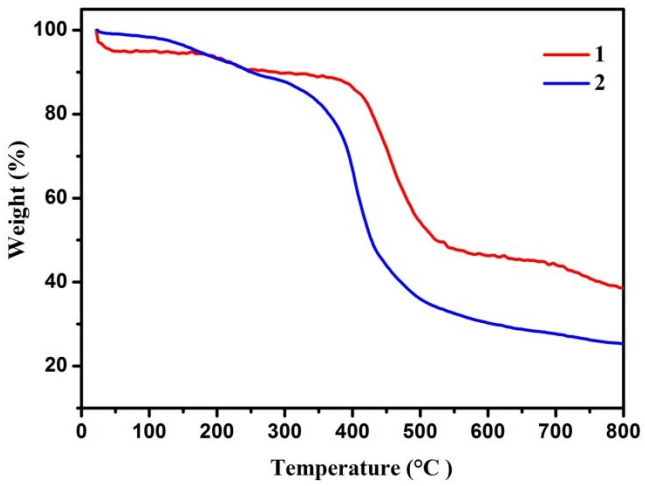


**Fig. S4** TG curves for **1** and **2**.

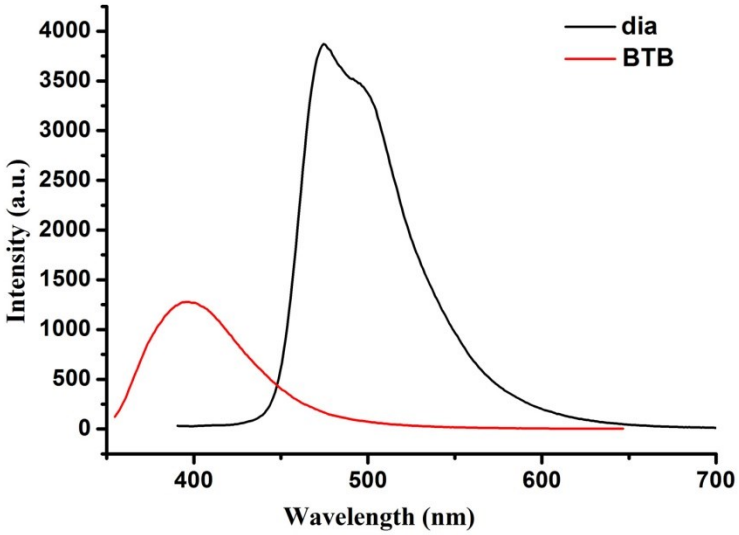


**Fig. S5** Emission spectra of btb and dia ligand.

**Table S1** Crystallographic data and structure refinements for **1** and **2.**

| | **1** | **2** |
|---|---|---|
| Formula | $C_{47}H_{30}N_4O_8Zn_2$ | $C_{74}H_{44}Cd_2N_4NaO_{12}$ |
| Mr | 909.53 | 1428.92 |
| Crystal system | triclinic | monoclinic |
| space group | P-1 | C2/c |
| a, Å | 9.797(4) | 32.143(4) |
| b, Å | 15.252(6) | 10.3824(10) |
| c, Å | 16.948(7) | 32.772(4) |
| α, deg | 75.387(7) | 90 |
| β, deg | 73.275(7) | 115.790(4) |
| γ, deg | 85.170(7) | 90 |
| V,Å$^3$ | 2346.7(16) | 9847.4(18) |
| Z | 2 | 4 |
| $D_X$, g cm$^{-3}$ | 1.287 | 0.964 |
| μ, mm$^{-1}$ | 1.075 | 0.480 |
| Unique. reflns/$R_{int}$ | 0.0577 | 0.0545 |
| $R_1$ [I>2σ(I)] | 0.0765 | 0.0721 |
| $wR_2$(All data) | 0.2153 | 0.2190 |
| GOF | 0.871 | 0.967 |

**Table S2** Selected bond lengths [Å] and Selected angles [°] for **1**.

| | | | |
|---|---|---|---|
| Zn1-N1 | 2.021(6) | O3#3-Zn2-O1#2 | 153.2(3) |
| Zn1-O2 | 1.945(4) | O3#3-Zn2-O9#2 | 92.47(16) |
| Zn1-O5#1 | 1.951(4) | O3#3-Zn2-N3 | 78.3(3) |
| Zn1-O9 | 1.934(4) | O9#2-Zn2-Zn2#2 | 84.6(3) |
| Zn2-O1#2 | 1.984(6) | O9-Zn2-O7 | 41.34(12) |
| Zn2-O3#3 | 1.969(4) | O9#2-Zn2-N3 | 88.19(18) |
| Zn2-O7 | 2.156(5) | N3-Zn2-Zn2#2 | 144.8(3) |
| Zn2-O9#2 | 2.109(4) | O2-Zn1-O5#1 | 120.92(18) |
| Zn2-O9 | 2.074(5) | O9-Zn1-N1 | 110.48(19) |
| Zn2-N3 | 2.327(8) | O9-Zn1-O5#1 | 109.68(18) |
| O2-Zn1-N1 | 98.6(2) | O1#2-Zn2-O7 | 86.4(2) |
| O5#1-Zn1-N1 | 107.4(2) | O1#2-Zn2-O9 | 109.5(2) |
| O9-Zn1-O2 | 108.96(17) | O3#3-Zn2-Zn2#2 | 96.18(15) |
| O1#2-Zn2-Zn2#2 | 106.59(19) | O3#3-Zn2-O7 | 89.50(19) |
| O1#2-Zn2-O9#2 | 95.37(19) | O3#3-Zn2-O9 | 96.8(2) |
| O1#2-Zn2-N3 | 74.9(3) | O7-Zn2-Zn2#2 | 130.37(15) |
| O9-Zn2-N3 | 83.53(17) | O9#2-Zn2-O7 | 42.19(10) |
| | | O9-Zn2-O9#2 | 171.66(19) |

Symmetry transformations used to generate equivalent atoms: [1]-1+X,+Y,1+Z; [2]-X,-Y,-1-Z; [3]1-X,-1-Y,-1-Z.

**Table S3** Selected bond lengths [Å] and Selected angles [°] for **2**.

| | | | |
|---|---|---|---|
| Cd1-O1#1 | 2.487(4) | O3-Cd1-O6#2 | 93.8(3) |
| Cd1-O2# | 2.277(4) | O3-Cd1-O8#2 | 147.9(3) |
| Cd1-N1 | 2.250(4) | O3-Cd1-N1 | 107.00(18) |
| Cd1-O3 | 2.167(5) | O3-Cd1-O6#2 | 93.8(3) |
| Cd1-O5#2 | 2.400(10) | O3-Cd1-O8#2 | 147.9(3) |
| Cd1-O6#2 | 2.358(8) | O3-Cd1-N1 | 107.00(18) |
| Cd1-O7#2 | 2.507(8) | O3-Cd1-O6#2 | 93.8(3) |
| Cd1-O8#2 | 2.384(11) | O3-Cd1-O8#2 | 147.9(3) |
| O1#1-Cd1-O7#2 | 139.4(3) | O2#1-Cd1-O1#1 | 54.02(13) |
| O2#1 Cd1-O5#2 | 108.6(3) | O2#1-Cd1-O6#2 | 113.4(3) |
| O2#1 Cd1-O7#2 | 86.3(3) | O2#1 Cd1 O8#2 | 88.8(3) |
| N1-Cd1-1#1 | 81.38(15) | N1-Cd1-O2#1 | 131.14(17) |
| N1-Cd1-O5#2 | 79.4(3) | N1-Cd1-O6#2 | 107.9(3) |
| N1-Cd1-O7#2 | 129.6(3) | N1-Cd1-O8#2 | 95.2(3) |
| O3-Cd1-O1#1 | 95.47(19) | O3-Cd1-O2#1 | 95.47(19) |
| O3-Cd1-N1 | 107.00(18) | O3-Cd1-O5#2 | 94.9(2) |
| | | O3-Cd1-O7#2 | 105.3(3) |

Symmetry transformations used to generate equivalent atoms:[1]+X,2-Y,1/2+Z; [2]-1/2+X,-1/2+Y,+Z.

**Table S4** The comparison of $K_{sv}$ for **1**, **2** and other reported MOFs.

| MOF | Ksv | Ref |
|---|---|---|
| 1 | $2.84\times10^5$ $M^{-1}$ | In this work |
| 2 | $2.50\times10^5 M^{-1}$ | In this work |
| [Tb(L)(OH)]· x(solv) | $7.73\times10\text{-}^2$ $ppm^{-1}$ | 1 |
| Zr-NDC/Tz and Zr-NDC/CN) | $1.8\times10^4 M^{-1}$ | 2 |
| $[Cd(NDC)_{0.5}(PCA)].xG$ | $3.5 \times 10^4$ $M^{-1}$ | 3 |
| $[(CH3)_2NH_2]3[Zn_4Na(BPTC)_3]\cdot4CH_3OH\cdot2DMF$ | $3.2\times10^4$ $M^{-1}$ | 4 |
| $[Zn(NDC)(H_2O)]n$ | $6 \times 10^4$ $M^{-1}$ | 5 |
| $[Cd(NDC)(H_2O)]n$ | $2.385 \times 10^4$ $M^{-1}$ | 5 |
| $\{[Tb(L)_{1.5}(H_2O)]\cdot3H_2O\}n$ | $7.47 \times 10^4$ $M^{-1}$ | 6 |

## Reference


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