

Structural diversity of metal-organic frameworks based on chalcone dicarboxylic acid

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Table S1 Crystalline data and structural parameters of compounds **1-3**.

Compounds	1	2	3
Empirical formula	C ₂₂ H ₁₈ O ₆ Zn	C ₂₂ H ₁₈ O ₆ Cd	C ₂₂ H ₁₈ O ₆ Cd
Formula weight	443.73	490.76	490.76
Temperature/K	296(2)	296(2)	296(2)
Crystal system	Triclinic	Triclinic	Monoclinic
Space group	<i>P</i> $\bar{1}$	<i>P</i> $\bar{1}$	<i>P</i> 2 ₁ / <i>n</i>
a/Å	5.9824(3)	5.9985(3)	5.99377(17)
b/Å	11.4997(5)	11.6150(9)	20.9969(6)
c/Å	14.2042(7)	14.3679(9)	14.6167(5)
α /°	106.267(4)	107.300(6)	90
β /°	99.849(4)	99.607(5)	96.052(3)
γ /°	98.211(4)	100.199(5)	90
Volume/Å ³	905.25(8)	914.62(11)	1829.27(10)
Z	2	2	4
$\rho_{\text{calc}}/\text{cm}^3$	1.628	1.782	1.782
μ/mm^{-1}	2.232	9.909	9.909
F(000)	456.0	492.0	984.0
Radiation	CuK α	CuK α	CuK α
Reflections collected	10194	5724	7178
Independent reflections	3489	3478	3530
R _{int}	0.0323	0.0335	0.0327
Goodness-of-fit on F ²	1.070	1.033	1.176
R ₁ ,wR ₂ [<i>I</i> ≥2 σ (<i>I</i>)]	0.0399, 0.1036	0.0321, 0.0773	0.0730, 0.1921

R₁, wR₂ [all data] 0.0452, 0.1089 0.0365, 0.0814 0.0819, 0.1999

^a R₁ = $\Sigma||F_o| - |F_c|| / \Sigma|F_o|$, ^b wR₂ = $\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]^{1/2}$.

Table S2 The primary bond length (Å) and bond angle (°) of compounds **1–3**.

Compound 1			
Zn1–O1	1.9505(17)	Zn1–O2	2.0777(19)
Zn1–O4	1.9928(19)	Zn1–O1W	2.0309(19)
Zn1–O3	2.443(2)	Zn1–C22#1	2.544(2)
O1–Zn1–O4	157.68(8)	O4–Zn1–O1W	91.58(8)
O1–Zn1–O3	116.66(8)	O4–Zn1–C22#1	29.21(9)
O1–Zn1–O2	99.14(7)	O3–Zn1–C22#1	28.96(8)
O1–Zn1–O1W	92.42(8)	O2–Zn1–O3	85.84(7)
O1–Zn1–C22#1	142.19(9)	O2–Zn1–C22#1	93.60(7)
O4–Zn1–O3	58.15(8)	O1W–Zn1–O3	149.57(7)
O4–Zn1–O2	101.92(8)	O1W–Zn1–O2	98.82(8)
O1W–Zn1–C22#1	120.67(9)		
Symmetry code: #1 +x, 1+y, -1+z			

Compound 2			
Cd1–O4#1	2.411(3)	Cd1–O2#3	2.350(3)
Cd1–O5#2	2.472(2)	Cd1–O1W	2.279(3)
Cd1–O1	2.205(3)	Cd1–C22#1	2.678(4)
Cd1–O3#1	2.263(3)	O2#3–Cd1–O4#1	83.99(9)
O4#1–Cd1–O5#2	82.93(9)	O2#3–Cd1–O5#2	160.41(10)
O4#1–Cd1–C22#1	28.16(11)	O2#3–Cd1–C22#1	92.31(10)
O5#2–Cd1–C22#1	82.92(9)	O1W–Cd1–O4#1	138.11(10)
O1–Cd1–O4#1	137.12(10)	O1W–Cd1–O5#2	103.40(11)
O1–Cd1–O5#2	80.83(10)	O1W–Cd1–O2#3	96.08(12)
O1–Cd1–O3#1	157.81(11)	O1W–Cd1–C22#1	110.52(11)
O1–Cd1–O2#3	99.21(10)	O3#1–Cd1–O5#2	84.49(9)

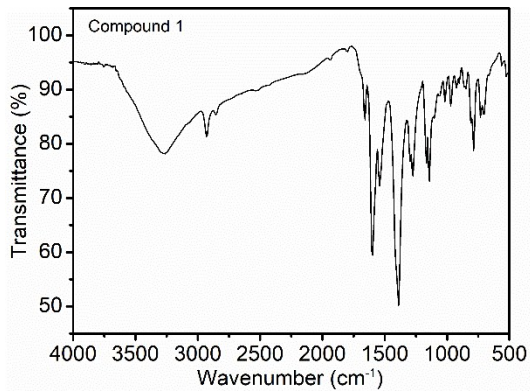
O1–Cd1–O1W	84.41(11)	O3#1–Cd1–O2#3	100.18(10)
O1–Cd1–C22#1	160.15(11)	O3#1–Cd1–O1W	82.92(10)
O3#1–Cd1–O4#1	56.17(9)	O3#1–Cd1–C22#1	28.00(11)

Symmetry codes: #1 +x, 1+y, -1+z; #2 1-x, 1-y, -z; #3 1-x, 2-y, -z.

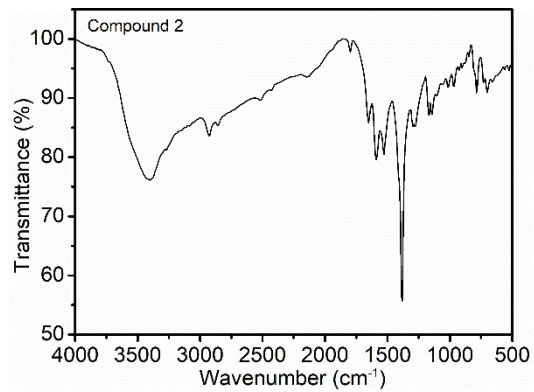
Compound 3

Cd1–O1	2.204(6)	Cd1–O3#1	2.425(5)
Cd1–O4#1	2.253(6)	Cd1–O5#3	2.479(6)
Cd1–O1W	2.272(6)	Cd1–C22#1	2.686(8)
Cd1–O2#2	2.348(6)	O4#1–Cd1–O5#3	84.05(19)
O1–Cd1–O4#1	157.8(2)	O1W–Cd1–O5#3	103.1(2)
O1–Cd1–O1W	85.1(2)	O2#2–Cd1–O5#3	160.3(2)
O4#1–Cd1–O1W	81.8(2)	O3#1–Cd1–O5#3	82.36(18)
O1–Cd1–O2#2	99.4(2)	O1–Cd1–C22#1	160.5(2)
O4#1–Cd1–O2#2	99.8(2)	O4#1–Cd1–C22#1	27.6(2)
O1W–Cd1–O2#2	96.5(2)	O1W–Cd1–C22#1	109.1(2)
O1–Cd1–O3#1	137.7(2)	O2#2–Cd1–C22#1	92.3(2)
O4#1–Cd1–O3#1	55.80(19)	O3#1–Cd1–C22#1	28.2(2)
O1W–Cd1–O3#1	136.76(19)	O5#3–Cd1–C22#1	82.20(19)
O2#2–Cd1–O3#1	83.94(19)	O1–Cd1–O5#3	81.6(2)

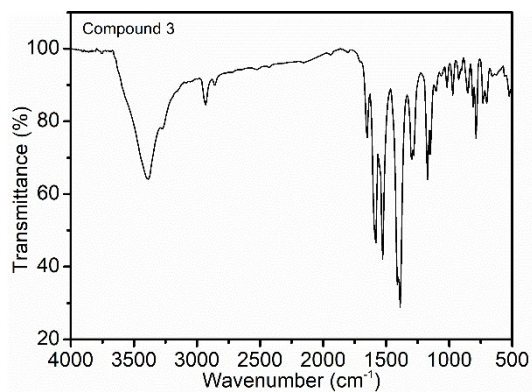
Symmetry codes: #1 +x, -1+y, +z; #2 1-x, -y, 1-z; #3 1/2-x, -1/2+y, 1/2-z.



(a)

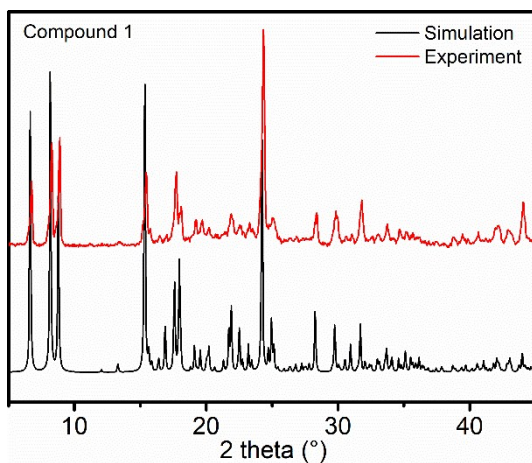


(b)

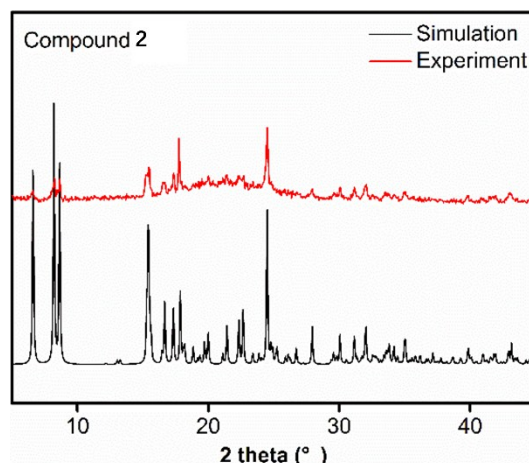


(c)

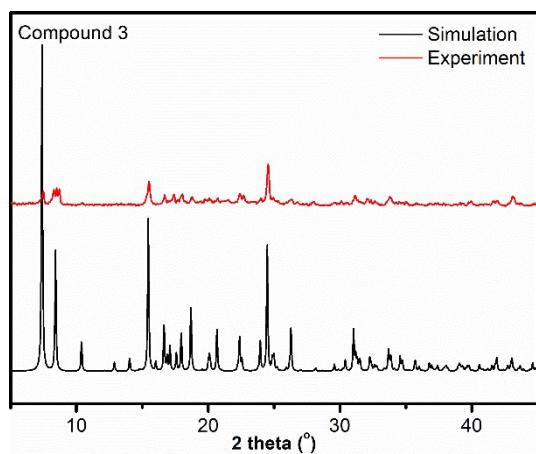
Fig. S1 IR spectra of compounds 1–3.



(a)



(b)



(c)

Fig. S2 The PXR D patterns of compounds 1–3.

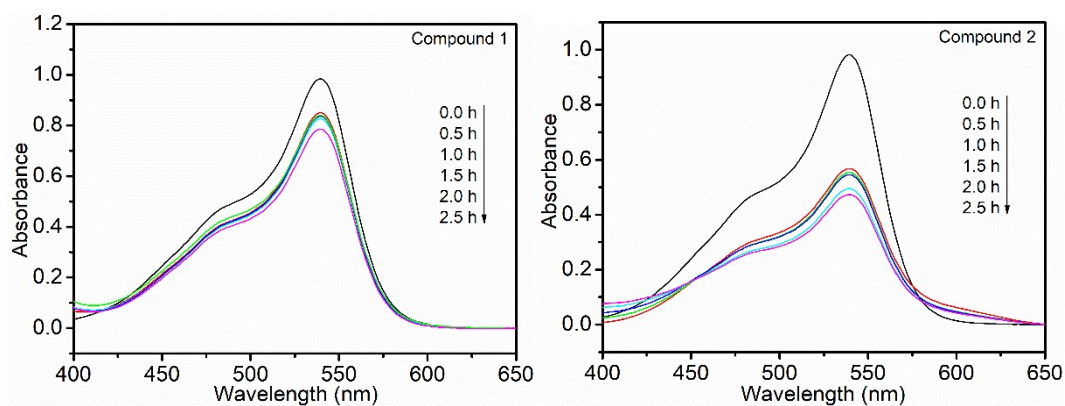


Fig. S3 Photocatalytic effects of compounds 1 and 2 on PH solution.

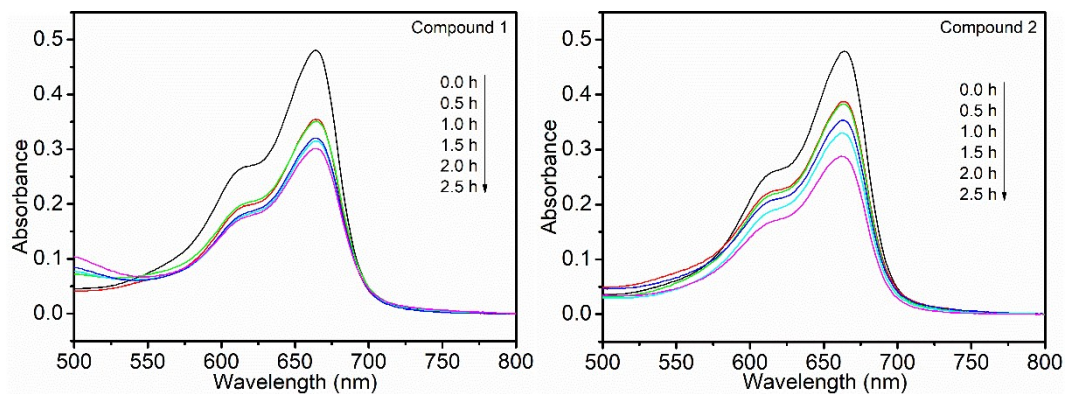


Fig. S4 Photocatalytic effects of compounds 1 and 2 on MB solution.