Experimental and Density Functional Theory Studies on Zinc(II) Coordination Polymer Constructed with 1, 3, 5-benzenetricarboxylic acid and the derived-nanocomposites from Activated Carbon

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Table S1. Crystal data and structure refinement for **$[Zn_3(BTC)_2(H_2O)_{12}]_n$,- ZnBTC.**

Table S2. Selected bond lengths for **$[Zn_3(BTC)_2(H_2O)_{12}]_n$,- ZnBTC.**

Table S3. Selected bond angles for **$[Zn_3(BTC)_2(H_2O)_{12}]_n$,- ZnBTC.**

Table S4. Fractional atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å2\times 10^3$) for **$[Zn_3(BTC)_2(H_2O)_{12}]_n$,- ZnBTC.** Ueq is defined as 1/3 of of the trace of the orthogonalized Uij tensor.

Table S5. Anisotropic displacement parameters ($Å^2\times 10^3$) for **$[Zn_3(BTC)_2(H_2O)_{12}]_n$,- ZnBTC.** The anisotropic displacement factor exponent takes the form :2π2[h2a*2u11+2hka*b*u12+…].

Table S6. Torsion Angles for **$[Zn_3(BTC)_2(H_2O)_{12}]_n$,- ZnBTC**.

Table S7. Hydrogen atom coordinates ($Å\times 10^4$) and isotropic displacement parameters ($Å^2\times 10^3$) for **$[Zn_3(BTC)_2(H_2O)_{12}]_n$,- ZnBTC.**

Table S1 Crystal data and structure refinement for $[Zn_3(BTC)_2(H_2O)_{12}]_n$,- ZnBTC.

CCDC 2053471	
Empirical formula	$C_{12}H_{20}O_{16}Zn_2$
Formula weight	551.02
Temperature/K	120.0(2)
Crystal system	Monoclinic
Space group	I2
a/Å	6.49670(10)
b/Å	12.92210(10)
c/Å	16.1403(2)
α/°	90
β/°	90.1460(10)
γ/°	90
Volume/Å^3	1354.99(3)
Z	3
ρ_{calc}g/cm^3	2.026
μ/mm^{-1}	4.104
F(000)	840.0
Crystal size/mm^3	0.232 × 0.076 × 0.054
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.766 to 146.358
Index ranges	$-8 \leq h \leq 7$, $-15 \leq k \leq 16$, $-20 \leq l \leq 20$
Reflections collected	9748
Independent reflections	2647 [R_{int} = 0.0163, R_{sigma} = 0.0113]
Data/restraints/parameters	2647/3/218
Goodness-of-fit on F^2	1.049
Final R indexes [I>=2σ (I)]	R_1 = 0.0217, wR_2 = 0.0561
Final R indexes [all data]	R_1 = 0.0218, wR_2 = 0.0561
Largest diff. peak/hole / e Å^{-3}	0.29/-0.41
Flack parameter	0.41(3)

Table S2 Bond Lengths for $[Zn_3(BTC)_2(H_2O)_{12}]_n$,- ZnBTC.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Zn1	O1	2.142(2)	Zn2	O9[1]	2.001(3)
Zn1	O2	2.098(2)	Zn2	O9	2.000(3)
Zn1	O3	2.150(2)	Zn2	C12	2.508(4)
Zn1	O4	2.111(2)	C3	C4	1.397(4)
Zn1	O5	2.040(2)	C4	C6	1.508(6)
Zn1	O10	2.041(2)	O5	C7	1.261(4)
C1	C2	1.502(4)	C6	O12	1.265(3)
C1	O10	1.262(4)	C6	O12[2]	1.265(3)
C1	O11	1.261(4)	O6	C7	1.264(4)
C2	C3	1.391(4)	O7	C12	1.271(3)
C2	C5	1.394(4)	C7	C8	1.512(4)
Zn2	O7	2.160(2)	C8	C9	1.388(4)
Zn2	O7[1]	2.160(2)	C8	C11	1.404(4)
Zn2	O8[1]	2.121(2)	C9	C10	1.392(4)
Zn2	O8	2.121(2)	C10	C12	1.481(6)

[1]1-x, +y,1-z; [2]1-x,+y, 2-z

Table S3 Bond Angles for $[Zn_3(BTC)_2(H_2O)_{12}]_n$,- ZnBTC.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Zn1	O3	177.19(10)	O9	Zn2	O8	84.80(10)
O2	Zn1	O1	90.17(9)	O9[1]	Zn2	O8	93.10(10)
O2	Zn1	O3	87.03(9)	O9[1]	Zn2	O8[1]	84.80(10)
O2	Zn1	O4	176.23(10)	O9	Zn2	O8[1]	93.10(10)
O4	Zn1	O1	93.57(9)	O9	Zn2	O9[1]	104.83(18)
O4	Zn1	O3	89.23(9)	O9[1]	Zn2	C12	127.58(9)
O5	Zn1	O1	89.08(9)	O9	Zn2	C12	127.58(9)
O5	Zn1	O2	85.89(9)	C2	C3	C4	120.0(3)
O5	Zn1	O3	90.59(9)	C3	C4	C3[2]	119.9(4)
O5	Zn1	O4	93.64(9)	C3	C4	C6	120.03(19)
O5	Zn1	O10	173.90(9)	C3[2]	C4	C6	120.03(19)
O10	Zn1	O1	85.98(9)	C2	C5	C2[2]	120.5(4)
O10	Zn1	O2	90.53(8)	C7	O5	Zn1	128.3(2)
O10	Zn1	O3	94.16(9)	O12	C6	C4	118.7(2)
O10	Zn1	O4	90.25(9)	O12[2]	C6	C4	118.7(2)
O10	C1	C2	116.7(3)	O12[2]	C6	O12	122.7(4)
O11	C1	C2	118.8(3)	C12	O7	Zn2	90.10(19)
O11	C1	O10	124.5(3)	O5	C7	O6	124.9(3)
C3	C2	C1	121.6(3)	O5	C7	C8	117.1(3)
C3	C2	C5	119.7(3)	O6	C7	C8	118.0(3)
C5	C2	C1	118.7(3)	C9	C8	C7	119.0(3)
O7[1]	Zn2	O7	60.89(12)	C9	C8	C11	119.7(3)
O7[1]	Zn2	C12	30.45(6)	C11	C8	C7	121.3(3)
O7	Zn2	C12	30.45(6)	C8	C9	C10	120.3(3)
O8	Zn2	O7	86.33(9)	C1	O10	Zn1	128.64(19)
O8[1]	Zn2	O7[1]	86.33(9)	C9[1]	C10	C9	120.1(4)
O8	Zn2	O7[1]	96.65(9)	C9[1]	C10	C12	119.9(2)
O8[1]	Zn2	O7	96.65(9)	C9	C10	C12	119.9(2)
O8[1]	Zn2	O8	176.56(13)	C8[1]	C11	C8	119.8(4)
O8	Zn2	C12	91.72(6)	O7	C12	Zn2	59.45(19)
O8[1]	Zn2	C12	91.72(6)	O7[1]	C12	Zn2	59.45(19)
O9	Zn2	O7[1]	97.98(11)	O7	C12	O7[1]	118.9(4)
O9[1]	Zn2	O7[1]	155.90(11)	O7[1]	C12	C10	120.55(19)
O9	Zn2	O7	155.90(11)	O7	C12	C10	120.55(19)
O9[1]	Zn2	O7	97.98(11)	C10	C12	Zn2	180.0

[1]1-x, +y, 1-z; [2]1-x, +y, 2-z

Table S4 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for [$Zn_3(BTC)_2(H_2O)_{12}]_n$,- ZnBTC. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*Z*	U(eq)
Zn1	5296.2(6)	6097.8(3)	7588.8(2)	8.84(12)
O1	2328(3)	6759.4(18)	7354.8(14)	13.4(4)
C1	5770(4)	8111(2)	8489.3(17)	9.0(5)
C2	5351(4)	8720(2)	9264.0(18)	8.3(6)
Zn2	5000	-1031.0(4)	5000	10.59(14)
O2	6637(4)	7158.3(16)	6767.6(14)	10.8(4)
C3	5350(4)	9796(3)	9264.1(19)	10.2(6)
O3	8338(4)	5485.5(18)	7780.2(14)	15.8(4)
C4	5000	10338(3)	10000	10.1(8)
O4	4136(4)	4980.5(17)	8420.0(14)	12.0(4)
C5	5000	8184(3)	10000	8.3(7)
O5	4909(3)	5170.8(17)	6577.0(13)	10.7(4)
C6	5000	11504(4)	10000	14.6(9)
O6	3707(3)	3722.2(16)	7163.8(13)	12.3(4)
O7	4553(3)	410.1(18)	5653.3(13)	11.5(4)
C7	4403(4)	4229(2)	6555.6(18)	9.3(6)
C8	4678(4)	3668(2)	5740.9(18)	9.4(6)
O8	7943(4)	-1080.3(18)	5570.9(15)	15.7(4)
C9	4651(5)	2594(2)	5733.8(18)	9.4(6)
O9	6252(4)	-1975(2)	4158.1(17)	24.4(6)
O10	5521(4)	7144.4(16)	8531.9(13)	11.5(4)
C10	5000	2056(3)	5000	9.5(8)
C11	5000	4212(3)	5000	8.3(7)
O11	6367(3)	8587.0(16)	7851.4(13)	12.3(4)
O12	4929(4)	11973.7(18)	10686.9(16)	21.6(6)
C12	5000	910(3)	5000	10.3(8)

Table S5 Anisotropic Displacement Parameters ($Å^2×10^3$) for $[Zn_3(BTC)_2(H_2O)_{12}]_n$,-ZnBTC. The Anisotropic displacement factor exponent takes the form: $2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Zn1	12.5(2)	6.62(19)	7.41(18)	-0.53(13)	0.12(13)	0.32(14)
O1	15.6(11)	10.3(10)	14.4(10)	-1.5(8)	0.0(8)	2.4(8)
C1	7.3(12)	10.3(13)	9.3(13)	0.4(11)	-1.8(10)	-0.8(11)
C2	6.3(13)	8.9(14)	9.7(14)	-1.4(10)	0.1(10)	-0.2(9)
Zn2	13.7(3)	7.5(3)	10.6(3)	0	-0.1(2)	0
O2	13.6(11)	8.4(10)	10.3(10)	-1.2(7)	1.6(8)	0.3(8)
C3	7.5(14)	10.9(14)	12.1(15)	2.2(11)	0.0(11)	-0.1(11)
O3	22.6(11)	12.2(11)	12.5(10)	-3.0(9)	-4.2(8)	6.4(9)
C4	6.7(18)	6(2)	18(2)	0	2.8(15)	0
O4	16.7(11)	9.3(10)	10.2(10)	-1.7(8)	2.9(8)	0.4(8)
C5	5.4(17)	6.7(18)	12.7(18)	0	-1.2(14)	0
O5	15.2(10)	7.0(10)	9.9(10)	-1.8(7)	0.3(8)	-1.1(8)
C6	12(2)	9(2)	23(2)	0	10.6(18)	0
O6	15.9(11)	10.1(10)	10.8(10)	-1.0(8)	3.1(8)	-2.9(8)
O7	15.8(10)	9.1(10)	9.8(10)	1.1(8)	1.7(8)	-0.3(8)
C7	6.6(13)	10.8(14)	10.6(13)	-0.6(11)	-1.0(10)	0.9(10)
C8	6.7(13)	10.7(14)	10.7(15)	-1.9(10)	-1.2(11)	0.0(10)
O8	15.1(10)	10.5(10)	21.4(11)	-3.2(9)	-5.1(9)	-0.2(9)
C9	8.4(14)	11.8(15)	8.1(14)	1.5(10)	1.1(11)	0.3(10)
O9	18.7(12)	27.2(14)	27.2(13)	-17.3(12)	-7.6(10)	5.9(11)
O10	17.5(12)	7.0(10)	10.1(10)	-0.6(7)	0.5(8)	-2.2(8)
C10	6.1(19)	9(2)	13(2)	0	-1.2(16)	0
C11	4.7(17)	8.4(18)	11.8(19)	0	-0.3(14)	0
O11	16.1(11)	11.2(10)	9.5(10)	-1.3(8)	3.0(8)	-2.6(8)
O12	26.3(13)	8.6(11)	30.1(14)	-5.5(10)	18.2(11)	-3.5(10)
C12	8.6(18)	12(2)	10.3(18)	0	-0.2(15)	0

Table S6 Torsion Angles for $[Zn_3(BTC)_2(H_2O)_{12}]_n$,- ZnBTC.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Zn1	O5	C7	O6	12.3(4)	O6	C7	C8	C9	-15.5(4)
Zn1	O5	C7	C8	-166.92(18)	O6	C7	C8	C11	165.8(2)
C1	C2	C3	C4	-178.6(2)	C7	C8	C9	C10	-176.9(2)
C1	C2	C5	C2[1]	178.6(3)	C7	C8	C11	C8[2]	177.7(3)
C2	C1	O10	Zn1	164.98(19)	C8	C9	C10	C9[2]	-0.9(2)
C2	C3	C4	C3[1]	0.0(2)	C8	C9	C10	C12	179.1(2)
C2	C3	C4	C6	180.0(2)	C9	C8	C11	C8[2]	-0.9(2)
Zn2	O7	C12	O7[2]	0.000(1)	C9[2]	C10	C12	O7	-175.43(18)
Zn2	O7	C12	C10	180.000(1)	C9	C10	C12	O7	4.57(18)
C3	C2	C5	C2[1]	0.0(2)	C9	C10	C12	O7[2]	-175.43(18)
C3	C4	C6	O12[1]	8.46(19)	C9[2]	C10	C12	O7[2]	4.57(18)
C3[1]	C4	C6	O12	8.46(19)	O10	C1	C2	C3	-172.7(3)
C3[1]	C4	C6	O12[1]	-171.54(19)	O10	C1	C2	C5	8.7(4)
C3	C4	C6	O12	-171.54(19)	C11	C8	C9	C10	1.8(4)
C5	C2	C3	C4	0.1(4)	O11	C1	C2	C3	8.3(4)
O5	C7	C8	C9	163.8(3)	O11	C1	C2	C5	-170.3(2)
O5	C7	C8	C11	-14.9(4)	O11	C1	O10	Zn1	-16.1(4)

[1]1-x, +y, 2-z; [2]1-x, +y, 1-z

Table S7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for $[Zn_3(BTC)_2(H_2O)_{12}]_n$,- ZnBTC.

Atom	*x*	*y*	*z*	U(eq)
H1A	2351.8	7405.82	7470.28	20
H1B	2067.11	6741.13	6835.18	20
H2A	7745.51	6905.27	6572.99	16
H2B	7024.65	7690.47	7036.08	16
H3	5587.27	10163.83	8763.61	12
H3A	8365.83	4846.22	7646.32	24
H3B	8626.42	5488.52	8297.22	24
H4A	3735.17	4448	8150.65	18
H4B	3042.73	5208.7	8649.04	18
H5	5000	7449.21	10000	10
H8A	8572.57	-617.93	5847.34	24
H8B	8733.27	-1603.6	5590.67	24
H9	4393.91	2224.47	6231.65	11
H9A	5539.36	-2365.72	3846.62	37
H9B	7373.56	-2301.17	4230.52	37
H11	5000.02	4947.4	5000	10