Support Information

The following are the detailed parameters of Zn-BTC, Co-BTC, and Zn-Co-BTC single crystals, in which Tables S3-1, S3-4, and S3-7 are crystal parameters, tables S3-2, S3-5, S3-8 and S3-3, S3-6, S3-9 are the intramolecular selective bond lengths and bond angles, respectively.

Table S3-1 Zn-BTC Crystal parameters

Formula	$C_{93}H_{92}Zn_{13}N_7O_{66}$
M/g·mol^{-1}	3213.54
T/K	193 K
Crystal system	orthorhombic
Space group	Cmc21
a/Å	29.577(8)
b/Å	28.974(8)
c/Å	17.758(5)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	15218(7)
Z	4
ρ_{calc}g/cm^3	1.403
Crystal size/mm^3	0.10 × 0.10 × 0.11
Reflections collected	2520
Final R indexes [I>=2σ (I)]	R_1 = 0.0567, wR_2 =0.3494
Final R indexes [all data]	R_1 = 0.0503, wR_2 = 0.1518
Refinement	SHELXL-97

Table S3-2 Selective bond lengths in Zn-BTC molecules

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Zn7	O30	2.089(7)	Zn4	O10	2.136(7)
Zn7	O31	2.058(9)	Zn4	O12	2.064(6)
Zn1	O17	2.171(6)	Zn5	O24	1.945(6)
Zn1	O3	2.098(5)	Zn5	O16	1.991(6)

Table S3-3 Selective bond angles in Zn-BTC molecules

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O30	Zn7	O23	89.4(2)	O23	Zn7	O28	89.5(3)
O30	Zn7	O28	92.5(2)	O28	Zn7	O28	85.1(5)
O30	Zn7	O30	176.4(4)	O3	Zn1	O17	91.8(2)
O31	Zn7	O23	88.2(3)	O5	Zn1	O17	175.2(2)
O31	Zn7	O28	90.2(3)	O5	Zn1	O3	92.8(2)
O23	Zn7	O23	95.9(4)	O25	Zn1	O17	87.5(3)

Table S3-4 Co-BTC Crystal parameters

Formula	$C_{45}H_{51}Co_3N_6O_{24}$
M/g·mol^{-1}	1236.71
T/K	296 K
Crystal system	monoclinic
Space group	P /21n
a/Å	16.6590(6)
b/Å	14.1439(5)
c/Å	28.8454(10)
α/°	90
β/°	90

γ/°	90
Volume/Å^3	6796.6(4)
Z	4
ρ_{calc}g/cm^3	1.209
Crystal size/mm^3	0.11 × 0.12 × 0.11
Reflections collected	1520
Final R indexes [I>=2σ (I)]	R_1 = 0.1353, wR_2 =0.3494
Final R indexes [all data]	R_1 = 0.0503, wR_2 = 0.1518
Refinement	SHELXL-97

Table S3-5 Selective bond lengths in Co-BTC molecules

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Co1	O2	2.361(13)	C1	O2	1.23(2)
Co1	O11	2.341(13)	C1	O1	1.28(2)
Co1	O9	2.460(12)	C1	C2	1.56(3)
Co1	O8	2.484(13)	C2	C3	1.39(6)

Table S3-6 Selective bond angles in Co-BTC molecules

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O2	Co1	O11	72.3(5)	O2	Co1	O12	72.7(4)
O2	Co1	O9	138.7(4)	O11	Co1	O12	72.9(4)
O11	Co1	O9	72.7(5)	O9	Co1	O12	76.7(4)
O2	Co1	O8	132.8(5)	O8	Co1	O12	138.3(4)
O11	Co1	O8	139.2(5)	O2	Co1	O7	72.6(4)
O9	Co1	O8	88.5(4)	O11	Co1	O7	144.5(5)

Table S3-7 Zn-Co-BTC Crystal parameters

Formula	$C_{102}H_{117}Co_2Zn_{12}N_{10}O_{74}$
M/g·mol^{-1}	3569.35
T/K	296
Crystal system	orthorhombic
Space group	Cmc21
a/Å	29.4994(10)
b/Å	28.8734(9)
c/Å	17.7149(6)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	15088.6(9)
Z	4
ρ_{calc}g/cm^3	1.571
Crystal size/mm^3	0.10× 0.12 × 0.12
Reflections collected	17235
Final R indexes [I>=2σ (I)]	R_1 = 0.0517, wR_2 = 0.1393
Final R indexes [all data]	R_1 = 0.0503, wR_2 = 0.1818
Refinement	SHELXL-97

Table S3-8 Selective bond lengths in Zn-Co-BTC molecules

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Zn1	O5	1.827(7)	Zn2	O1	2.099(6)
Zn1	O7	2.055(8)	Zn2	O8	2.083(7)
Zn1	O8	1.990(7)	Zn2	O9	2.053(8)
Zn1	O11	1.968(14)	Zn2	O10	2.083(5)

Table S3-9 Selective bond angles in Zn-Co-BTC molecules

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O5	Zn1	Zn1	107.4(3)	O8	Zn1	O7	116.9(3)
O5	Zn1	O7	102.8(3)	O11	Zn1	Zn1	146.0(4)
O5	Zn1	O8	127.7(3)	O11	Zn1	O7	91.8(7)
O5	Zn1	O11	105.9(5)	O11	Zn1	O8	105.4(5)
O7	Zn1	Zn1	74.1(3)	O1	Zn2	O1	83.7(4)
O8	Zn1	Zn1	58.01(13)	O8	Zn2	O1	92.4(2)

Figure S1(a) (b) (c) (d) were the relationship between the decomposition temperature and the heating rate of pure AP and after adding 10 wt.% catalysts Zn-BTC, Co-BTC, Zn-Co-BTC respectively. The corresponding activation energies can be calculated.

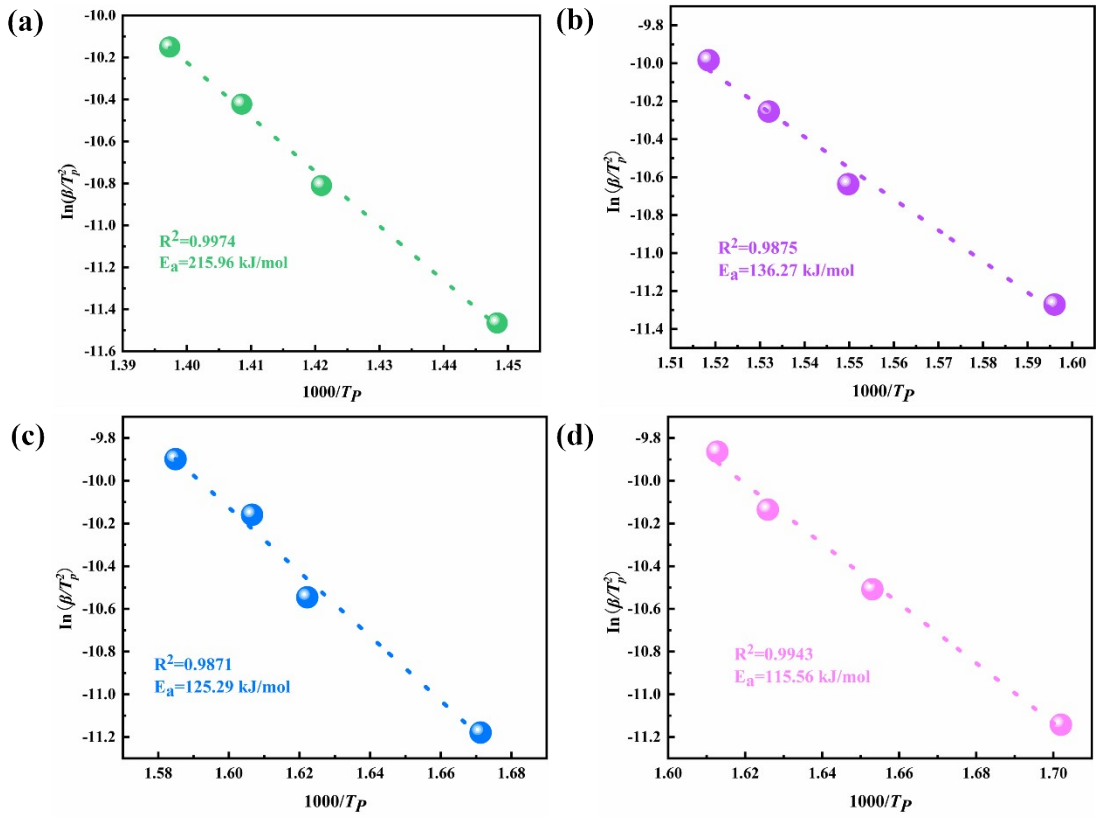

Fig.S1 (a) Dependence of $ln(\beta/T_P^2)$ on 1000/Tp during AP decomposition; (b-d) Dependence of $ln(\beta/T_P^2)$ on 1000/Tp during AP decomposition with the addition of Zn-BTC Co-BTC and Zn-Co-BTC (at 10 wt.% mass basis)