Green Bismuth Metal-Organic Framework Catalyzing RDX Combustion and Thermal Decomposition

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Table S1 Bond Lengths [Å] for $[Bi_2(pzdc)_4]\cdot 2DMF$.

Bi1 - O101	2.717(10)	C(1)-C(6)	1.516(4)
Bi1 - O121	2.737(10)	C(1)-C(8)	1.390(5)
Bi1 - O122	2.575(9)	C(2)-H(2A)	0.9600
Bi1 - O8	2.314(8)	C(2)-H(2B)	0.9600
Bi1 - O1	2.410(9)	C(2)-H(2C)	0.9600
Bi1 - O13	2.220(10)	C(3)-H(3)	0.9300
Bi1 - N4	2.537(11)	C(3)-C(5)	1.383(6)
Bi1 - N1	2.554(10)	C(3)-C(10)	1.373(6)
Bi2 - O15	2.411(11)	C(4)-C(4)#4	1.495(6)
Bi2 - O9	2.410(8)	C(4)-C(5)	1.389(5)
Bi2 - O52	2.429(9)	C(5)-H(5)	0.9300
Bi2 - O63	2.644(11)	C(7)-H(7)	0.9300
Bi2 - N5	2.552(10)	C(8)-H(8)	0.9300
Bi2 - N22	2.655(10)	C(8)-C(10)	1.373(5)
Bi2 - C28	2.808(16)	C(9)-H(9A)	0.9600
Bi2 - O16	2.561(14)	C(9)-H(9B)	0.9600
Bi2 - O44	2.458(10)	C28 - O16	1.271(19)
Bi2 - O34	2.690(11)	C20 - C15	1.498(17)
O14 - C27	1.203(18)	C20 - Bi4	2.857(18)
O15 - C28	1.21(2)	C21 - C16	1.51(2)
O9 - C20	1.226(16)	C16 - C15	1.366(17)
O9 - Bi4	2.047(16)	C16 - N17	1.355(16)
O10 - C20	1.267(15)	C19 - C18	1.390(17)
O12 - C21	1.232(18)	C18 - N17	1.327(15)
O12 - Bi35	2.520(11)	C7 - C2	1.539(18)

O11 - C21	1.236(18)	C7 - O4	1.189(18)
O5 - C13	1.252(13)	C7 - O3	1.242(19)
O6 - C13	1.252(13)	C14 - C9	1.48(2)
O6 - Bi41	1.95(2)	C9 - N10	1.346(18)
O8 - C14	1.236(16)	C9 - C8	1.373(17)
O8 - Bi3	2.551(12)	N10 - C11	1.35(2)
O7 - C14	1.244(19)	C11 - C12	1.40(2)
O1 - C6	1.225(16)	C8 - C13	1.529(15)
O1 - Bi3	2.478(12)	C6 - C1	1.49(2)
O2 - C6	1.212(17)	C1 - C2	1.406(18)
O13 - C27	1.302(17)	C5 - C4	1.393(17)
O13 - Bi3	1.574(13)	C4 - N3	1.32(2)
N4 - C22	1.286(18)	N3 - C2	1.35(2)
N4 - C26	1.281(17)	O3 - Bi46	2.508(16)
N4 - Bi3	2.177(14)		
[1]3/2-X,1/2+Y,3/2-Z; [2]-1/2+X,1/2-Y,-1/2+Z; [3]3/2-X,-1/2+Y,3/2-Z; [4]1/2+X,1/2-Y,-1/2+Z; [5]1/2+X,1/2-Y,1/2+Z; [6]-1/2+X,1/2-Y,1/2+Z			

Table S2 Bond Angles [°] for $[Bi_2(pzdc)_4]\cdot 2DMF$.

O101-Bi1-O121	64.6(3)	O13-C27-C22	115.7(12)
O122-Bi1-O101	112.9(3)	O13-C27-Bi3	36.1(6)
O122-Bi1-O121	70.3(4)	C22-C27-Bi3	80.9(8)
O8-Bi1-O101	73.3(3)	N4-C22-C27	117.7(12)
O8-Bi1-O122	143.8(3)	N4-C22-C23	123.8(13)
O8-Bi1-O121	82.2(3)	N4-C22-Bi3	53.9(7)
O8-Bi1-O1	143.7(3)	C27-C22-Bi3	63.9(7)
O8-Bi1-N4	73.8(3)	C23-C22-C27	118.1(12)
O8-Bi1-N1	78.1(3)	C23-C22-Bi3	171.1(10)
O1-Bi1-O101	93.5(3)	N4-C26-C25	124.0(15)
O1-Bi1-O121	123.1(3)	C24-C25-C26	117.3(15)
O1-Bi1-O122	72.5(3)	C23-C24-C25	120.9(13)
O1-Bi1-N4	133.7(4)	C22-C23-C28	127.2(14)

O1-Bi1-N1	65.6(3)	C24-C23-C22	115.5(13)
O13-Bi1-O101	145.6(3)	C24-C23-C28	116.6(13)
O13-Bi1-O122	98.1(4)	O15-C28-Bi2	58.7(8)
O13-Bi1-O121	144.6(3)	O15-C28-C23	120.7(14)
O13-Bi1-O8	90.7(4)	O15-C28-O16	124.4(16)
O13-Bi1-O1	81.5(4)	C23-C28-Bi2	173.1(11)
O13-Bi1-N4	69.6(3)	O16-C28-Bi2	65.7(9)
O13-Bi1-N1	73.5(4)	O16-C28-C23	114.5(16)
N4-Bi1-O101	130.4(3)	O9-C20-O10	122.1(12)
N4-Bi1-O122	76.6(3)	O9-C20-C15	121.1(11)
N4-Bi1-O121	75.2(3)	O9-C20-Bi4	38.6(6)
N4-Bi1-N1	132.6(4)	O10-C20-C15	116.7(12)
N1-Bi1-O101	73.5(3)	O10-C20-Bi4	153.7(11)
N1-Bi1-O121	137.2(3)	C15-C20-Bi4	84.8(7)
N1-Bi1-O122	138.0(3)	O12-C21-O11	125.9(16)
O15-Bi2-O52	102.8(4)	O12-C21-C16	117.2(13)
O15-Bi2-O63	144.8(3)	O11-C21-C16	116.8(15)
O15-Bi2-N5	71.3(4)	C15-C16-C21	127.8(12)
O15-Bi2-N22	120.5(4)	N17-C16-C21	112.0(11)
O15-Bi2-C28	25.5(4)	N17-C16-C15	119.7(11)
O15-Bi2-O16	52.4(4)	N5-C15-C20	114.7(11)
O15-Bi2-O44	72.5(4)	N5-C15-C16	123.1(12)
O15-Bi2-O34	119.0(4)	C16-C15-C20	122.2(11)
O9-Bi2-O15	75.2(4)	N5-C19-C18	121.5(12)
O9-Bi2-O52	136.5(3)	N17-C18-C19	120.9(11)
O9-Bi2-O63	81.4(3)	C18-N17-C16	118.0(11)
O9-Bi2-N5	65.7(3)	O4-C7-C2	121.2(15)
O9-Bi2-N22	153.9(3)	O4-C7-O3	121.0(14)
O9-Bi2-C28	99.9(4)	O3-C7-C2	117.7(14)
O9-Bi2-O16	125.9(4)	C28-O16-Bi2	87.4(11)
O9-Bi2-O44	77.0(4)	O8-C14-O7	126.1(15)
O9-Bi2-O34	78.1(3)	O8-C14-C9	118.3(14)

O52-Bi2-O63	76.9(3)	O7-C14-C9	114.9(13)
O52-Bi2-N5	72.5(3)	N10-C9-C14	116.6(11)
O52-Bi2-N22	64.4(3)	N10-C9-C8	119.7(12)
O52-Bi2-C28	89.1(4)	C8-C9-C14	123.6(12)
O52-Bi2-O16	74.6(4)	C11-N10-C9	118.0(13)
O52-Bi2-O44	145.0(4)	N10-C11-C12	120.7(14)
O52-Bi2-O34	133.0(3)	N2-C12-C11	121.6(13)
O63-Bi2-N22	91.6(3)	N2-C8-C9	122.9(12)
O63-Bi2-C28	160.0(4)	N2-C8-C13	113.7(10)
O63-Bi2-O34	80.4(3)	C9-C8-C13	123.4(11)
N5-Bi2-O63	75.2(3)	O5-C13-C8	117.7(9)
N5-Bi2-N22	136.7(3)	O6-C13-O5	125.5(10)
N5-Bi2-C28	87.0(4)	O6-C13-C8	116.8(10)
N5-Bi2-O16	103.6(4)	O1-C6-C1	117.1(12)
N5-Bi2-O34	138.7(4)	O2-C6-O1	129.0(15)
N22-Bi2-C28	95.2(4)	O2-C6-C1	113.9(13)
N22-Bi2-O34	75.9(3)	N1-C1-C6	117.5(11)
O16-Bi2-O63	150.3(4)	N1-C1-C2	116.3(12)
O16-Bi2-N22	68.6(4)	C2-C1-C6	126.2(12)
O16-Bi2-C28	26.9(4)	N1-C5-C4	118.2(12)
O16-Bi2-O34	113.8(4)	N3-C4-C5	126.5(13)
O44-Bi2-O63	127.1(4)	C4-N3-C2	112.7(12)
O44-Bi2-N5	133.2(4)	C1-C2-C7	122.8(13)
O44-Bi2-N22	87.7(4)	N3-C2-C7	111.4(11)
O44-Bi2-C28	72.1(4)	N3-C2-C1	125.8(13)
O44-Bi2-O16	75.8(4)	C7-O4-Bi26	100.2(10)
O44-Bi2-O34	48.3(4)	C7-O3-Bi26	87.5(9)
O34-Bi2-C28	119.5(4)	C7-O3-Bi46	99.1(10)
C28-O15-Bi2	95.8(10)	O122-Bi3-O8	132.8(5)
C20-O9-Bi2	122.1(8)	O122-Bi3-N1	131.0(5)
C20-O9-Bi4	119.5(9)	O122-Bi3-C22	95.9(5)
C20-O10-Bi13	116.7(9)	O8-Bi3-N1	70.9(4)

Bi15-O12-Bi13	109.7(4)	O8-Bi3-C22	86.7(4)
C21-O12-Bi13	124.1(9)	O1-Bi3-O122	72.4(4)
C21-O12-Bi15	116.6(10)	O1-Bi3-O8	126.4(5)
[1]3/2-X,1/2+Y,3/2-Z; [2]-1/2+X,1/2-Y,-1/2+Z; [3]3/2-X,-1/2+Y,3/2-Z; [4]1/2+X,1/2-Y,-1/2+Z; [5]1/2+X,1/2-Y,1/2+Z; [6]-1/2+X,1/2-Y,1/2+Z			

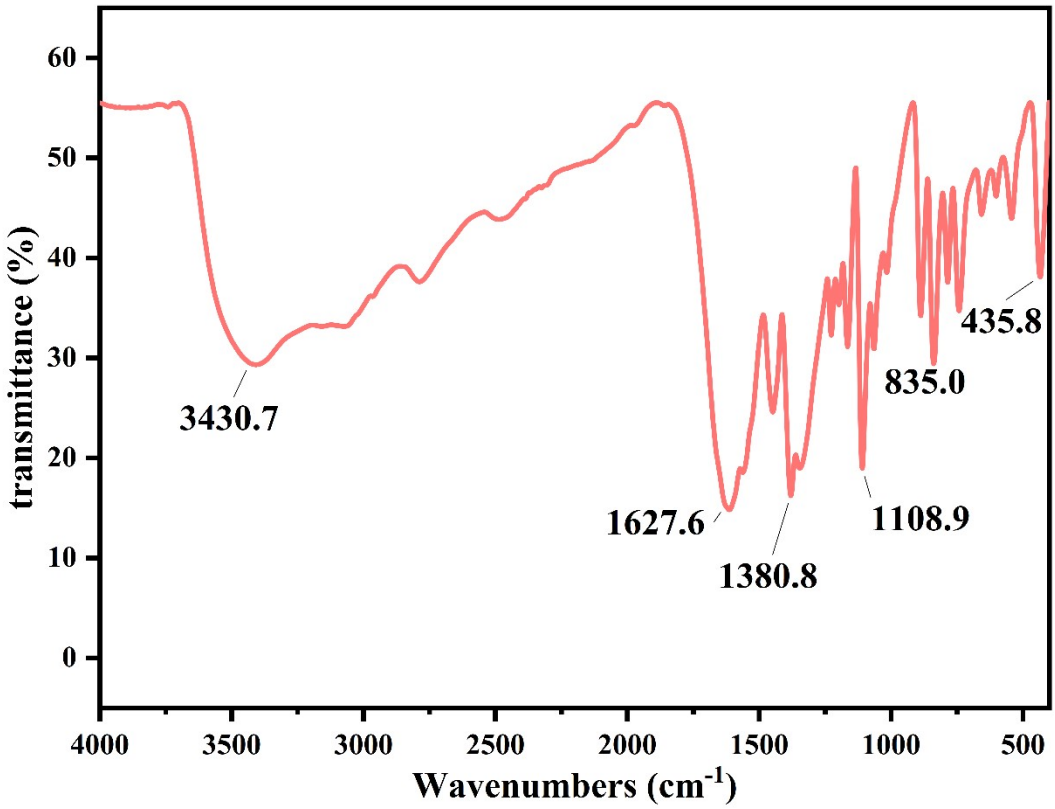

Fig. S1 FTIR spectra of $[Bi_2(pzdc)_4]\cdot 2DMF$.

As shown in Fig. S1, the FTIR spectrum of $[Bi_2(pzdc)_4]\cdot 2DMF$ in the 400–4000 cm^{-1} range exhibits characteristic peaks associated with its structure: the asymmetric stretching vibration ($\nu_{as}(COO^-)$) of carboxylate groups is observed at 1627.6 cm^{-1}, and the symmetric stretching vibration ($\nu_s(COO^-)$) appears at 1380.8 cm^{-1}. Additionally, absorption peaks in the low-wavenumber region (835.0 cm^{-1} and 435.8 cm^{-1}) are attributed to the stretching or bending vibrations of Bi–O coordination bonds. These features provide direct evidence for the coordination between carboxylate oxygen atoms and Bi^{3+} ions, confirming the formation of the MOF.

Table S3 Kinetic parameters of $[Bi_2(pzdc)_4]\cdot 2DMF$+RDX and pure RDX.

Samples	$[Bi_2(pzdc)_4]\cdot 2DMF$+RDX	Pure RDX
E_K(kJ/mol)	148.18	167.37
ln$A$	27.47	31.97
R_K	0.9886	0.9954
E_o (kJ/mol)	149.00	167.28

R_o	0.9897	0.9958