

Three Novel Green Bismuth-Based Combustion Catalysts for Catalyzing the High-Energy Oxidizer RDX

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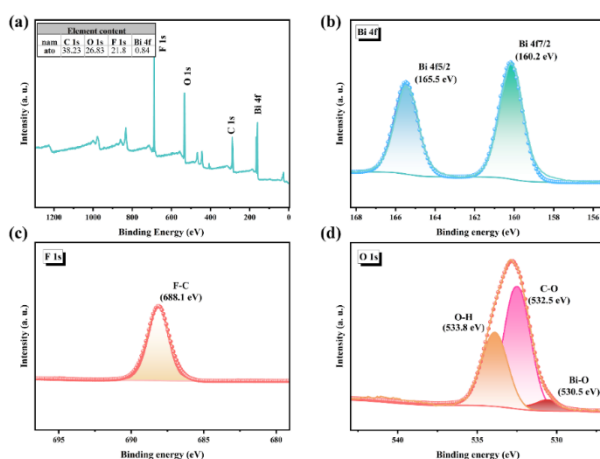


Fig. S1. XPS spectra of $[\text{BiO}(\text{TFPHA})\text{H}_2\text{O}] \cdot \text{H}_2\text{O}$: (a) survey, (b) Bi 4f5/2, (c) O 1s, and (d) C 1s.

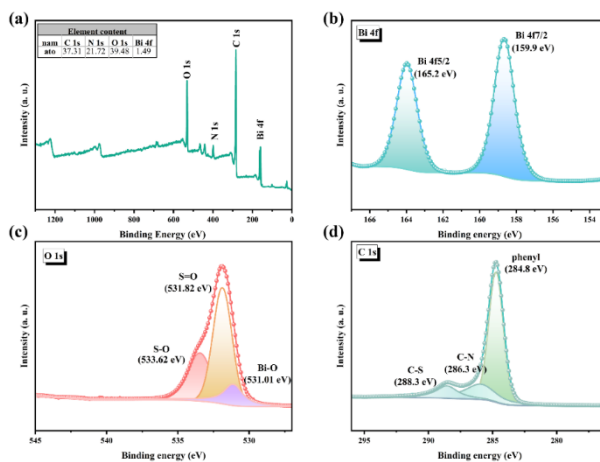


Fig. S2. XPS spectra of $[\text{Bi}(\text{BPSA})(\text{PHON})(\text{Ph})] \cdot 3\text{DMF}$: (a) survey, (b) Bi 4f5/2, (c) F 1s, and (d) O 1s.

Table S1 Bond Lengths [Å] for $[\text{Bi}_2(\text{DHBQDC})(\text{OX})_2(\text{DMF})_6]$

Bi1 - O61	2.414(5)	C3 - C2	1.405(12)
Bi1 - O5	2.402(5)	C5 - C52	1.524(16)
Bi1 - O82	2.511(5)	N3 - C7	1.268(17)
Bi1 - O7	2.324(6)	N3 - C9	1.493(9)
Bi1 - O33	2.627(6)	N3 - C8	1.487(9)
Bi1 - O11	2.457(7)	C4 - C2	1.404(12)

Bi1 - O4	2.638(6)	C2 - C1	1.419(16)
Bi1 - O9	2.477(6)	N1 - C13	1.302(14)
Bi1 - O10	2.685(8)	N1 - C15	1.398(17)
O6 - C6	1.240(9)	N1 - C14	1.417(17)
O10 - C10	1.198(14)	N3A - C9A	1.454(15)
C3 - C43	1.529(14)	N3A - C8A	1.447(16)
¹ -X,1-Y,1-Z; ² -X,1-Y,-Z; ³ 1-X,1-Y,1-Z			

Table S2 Bond Angles [°] for [Bi₂(DHBQDC)(OX)₂(DMF)₆]

O61-Bi1-O82	133.76(19)	C7-O11-Bi1	131.0(8)
O61-Bi1-O33	95.0(2)	C3-O4-Bi1	118.5(6)
O61-Bi1-O11	140.7(2)	C13-O9-Bi1	132.0(7)
O61-Bi1-O4	67.8(2)	O6-C6-O5	125.7(8)
O61-Bi1-O9	73.4(2)	O6-C6-C61	116.8(9)
O61-Bi1-O10	132.4(2)	O5-C6-C61	117.5(9)
O5-Bi1-O61	67.61(19)	C10-O10-Bi1	130.6(8)
O5-Bi1-O82	129.70(19)	O4-C3-C43	115.2(9)
O5-Bi1-O33	70.6(2)	O4-C3-C2	126.5(9)
O5-Bi1-O11	73.3(2)	C2-C3-C43	118.3(8)
O5-Bi1-O4	107.5(2)	O8-C5-O7	124.5(7)
O5-Bi1-O9	136.2(2)	O8-C5-C52	117.8(9)
O5-Bi1-O10	133.9(2)	O7-C5-C52	117.7(9)
O82-Bi1-O33	130.2(2)	C7-N3-C9	134(2)
O82-Bi1-O4	122.6(2)	C7-N3-C8	112(2)
O82-Bi1-O10	71.4(2)	C8-N3-C9	113.4(10)
O7-Bi1-O61	79.0(2)	O3-C4-C33	117.8(8)
O7-Bi1-O5	77.3(2)	O3-C4-C2	124.3(10)
O7-Bi1-O82	67.57(19)	C2-C4-C33	117.7(9)
O7-Bi1-O33	147.1(2)	C3-C2-C1	117.2(9)
O7-Bi1-O11	89.3(2)	C4-C2-C3	123.9(10)
O7-Bi1-O4	140.3(2)	C4-C2-C1	118.9(10)
O7-Bi1-O9	76.4(2)	C13-N1-C15	125.8(14)
O7-Bi1-O10	139.0(2)	C13-N1-C14	119.5(13)
O33-Bi1-O4	60.1(2)	C15-N1-C14	114.7(12)
O33-Bi1-O10	66.9(3)	C10-N2-C12	119.5(11)
O11-Bi1-O82	71.5(2)	C10-N2-C11	122.2(12)
O11-Bi1-O33	74.9(2)	C11-N2-C12	118.3(11)

O11-Bi1-O4	130.2(2)	O1-C1-C2	121.3(12)
O11-Bi1-O9	140.1(2)	O1-C1-O2	119.2(14)
O11-Bi1-O10	79.1(3)	O2-C1-C2	119.2(12)
O4-Bi1-O10	65.1(2)	O1A-C1-C2	114(4)
O9-Bi1-O82	68.5(2)	O1A-C1-O2A	127(3)
O9-Bi1-O33	133.3(2)	O2A-C1-C2	119(3)
O9-Bi1-O4	73.9(2)	O9-C13-N1	127.5(13)
O9-Bi1-O10	87.6(3)	O10-C10-N2	126.2(13)
C6-O6-Bi11	118.9(5)	O11-C7-N3	139.6(19)
C6-O5-Bi1	118.8(5)	O11-C7-N3A	137.5(16)
C5-O8-Bi12	114.2(5)	C7-N3A-C9A	133(2)
C5-O7-Bi1	119.9(5)	C7-N3A-C8A	112.1(19)
C4-O3-Bi13	116.5(6)	C8A-N3A-C9A	114.0(17)
¹ -X,1-Y,1-Z; ² -X,1-Y,-Z; ³ 1-X,1-Y,1-Z			

Table S3 Bond Lengths [Å] for [Bi(BPSA)(PHON)(Ph)]·3DMF

Bi1 - O1	2.526(4)	C13 - C14	1.385(8)
Bi1 - O51	2.455(3)	C13 - C18	1.374(7)
Bi1 - N1	2.426(4)	C14 - C15	1.371(9)
Bi1 - N2	2.467(4)	C15 - C16	1.340(10)
Bi1 - C13	2.260(5)	C16 - C17	1.360(11)
S1 - O1	1.474(4)	C17 - C18	1.414(8)
S1 - O2	1.431(4)	C19 - C31	1.321(14)
S1 - O3	1.452(4)	C19 - C34	1.422(12)
S1 - C19	1.767(5)	C19 - C20	1.337(11)
S2 - O4	1.448(4)	C19 - C24	1.391(10)
S2 - O5	1.481(4)	C22 - C25	1.479(7)
S2 - O6	1.429(4)	C22 - C32	1.311(14)
S2 - C28	1.769(5)	C22 - C33	1.435(13)
N1 - C1	1.278(7)	C22 - C21	1.349(10)
N1 - C12	1.378(6)	C22 - C23	1.418(10)
N2 - C10	1.320(7)	C25 - C26	1.386(8)
N2 - C11	1.354(6)	C25 - C30	1.369(7)
C1 - C2	1.426(8)	C26 - C27	1.372(8)
C2 - C3	1.317(9)	C27 - C28	1.360(7)
C3 - C4	1.403(9)	C28 - C29	1.360(7)
C4 - C5	1.461(9)	C29 - C30	1.391(7)

C4 - C12	1.401(7)	C31 - C32	1.406(14)
C5 - C6	1.349(9)	C33 - C34	1.391(13)
C6 - C7	1.384(8)	O7 - C35	1.167(11)
C7 - C8	1.392(9)	N3 - C35	1.250(12)
C7 - C11	1.432(7)	N3 - C36	1.423(11)
C8 - C9	1.339(9)	N3 - C37	1.454(12)
C9 - C10	1.415(9)	C20 - C21	1.408(12)
C11 - C12	1.429(7)	C23 - C24	1.386(12)
¹ /2-X,-1/2+Y,3/2-Z			

Table S4 Bond Angles [°] for [Bi(BPSA)(PHON)(Ph)]·3DMF

O51-Bi1-O1	132.89(12)	C12-C11-C7	119.5(5)
O51-Bi1-N2	151.62(13)	N1-C12-C4	121.0(5)
N1-Bi1-O1	139.90(14)	N1-C12-C11	119.0(4)
N1-Bi1-O51	83.59(13)	C4-C12-C11	119.9(5)
N1-Bi1-N2	68.03(15)	C14-C13-Bi1	120.9(4)
N2-Bi1-O1	74.46(13)	C18-C13-Bi1	120.5(4)
C13-Bi1-O1	84.20(16)	C18-C13-C14	118.5(5)
C13-Bi1-O51	85.00(17)	C15-C14-C13	120.8(7)
C13-Bi1-N1	83.35(15)	C16-C15-C14	120.7(7)
C13-Bi1-N2	91.83(18)	C15-C16-C17	120.7(7)
O1-S1-C19	104.9(2)	C16-C17-C18	119.5(7)
O2-S1-O1	113.1(3)	C13-C18-C17	119.7(6)
O2-S1-O3	115.4(2)	C31-C19-S1	123.3(7)
O2-S1-C19	107.1(2)	C31-C19-C34	117.2(9)
O3-S1-O1	108.0(2)	C34-C19-S1	118.1(6)
O3-S1-C19	107.6(3)	C20-C19-S1	120.9(6)
O4-S2-O5	110.7(2)	C20-C19-C24	120.2(7)
O4-S2-C28	105.3(2)	C24-C19-S1	118.9(5)
O5-S2-C28	105.3(2)	C32-C22-C25	124.1(8)
O6-S2-O4	115.0(3)	C32-C22-C33	117.6(10)
O6-S2-O5	112.7(2)	C33-C22-C25	117.7(7)
O6-S2-C28	107.0(2)	C21-C22-C25	123.4(6)
S1-O1-Bi1	106.4(2)	C21-C22-C23	116.3(7)
S2-O5-Bi12	118.14(19)	C23-C22-C25	120.2(6)
C1-N1-Bi1	123.6(4)	C26-C25-C22	121.2(5)

C1-N1-C12	119.1(5)	C30-C25-C22	121.7(5)
C12-N1-Bi1	117.3(3)	C30-C25-C26	117.1(5)
C10-N2-Bi1	124.4(4)	C27-C26-C25	121.7(6)
C10-N2-C11	117.6(5)	C28-C27-C26	120.3(6)
C11-N2-Bi1	117.2(4)	C27-C28-S2	119.9(4)
N1-C1-C2	122.6(6)	C29-C28-S2	120.7(4)
C3-C2-C1	119.6(6)	C29-C28-C27	119.1(5)
C2-C3-C4	120.0(6)	C28-C29-C30	120.7(5)
C3-C4-C5	123.6(6)	C25-C30-C29	120.9(5)
C12-C4-C3	117.7(6)	C19-C31-C32	120.6(14)
C12-C4-C5	118.7(6)	C22-C32-C31	123.3(14)
C6-C5-C4	119.9(6)	C34-C33-C22	118.2(11)
C5-C6-C7	123.0(6)	C33-C34-C19	121.0(11)
C6-C7-C8	124.9(6)	C35-N3-C36	119.0(9)
C6-C7-C11	119.0(6)	C35-N3-C37	119.8(11)
C8-C7-C11	116.1(6)	C36-N3-C37	121.2(11)
C9-C8-C7	122.2(7)	O7-C35-N3	127.0(12)
C8-C9-C10	117.4(7)	C19-C20-C21	119.7(10)
N2-C10-C9	124.1(6)	C22-C21-C20	122.8(10)
N2-C11-C7	122.4(5)	C24-C23-C22	121.3(8)
N2-C11-C12	118.1(5)	C23-C24-C19	119.2(8)
¹ 1/2-X,-1/2+Y,3/2-Z; ² 1/2-X,1/2+Y,3/2-Z			

Table S5 Bond Lengths [Å] for [BiO(TFPHA)H₂O]·H₂O

Bi1 - Bi11	3.6421(4)	O1 - C1	1.247(7)
Bi1 - O1	2.434(4)	O2 - C1	1.263(7)
Bi1 - O22	2.624(4)	O3 - C8	1.245(7)
Bi1 - O33	2.686(4)	O4 - C8	1.257(7)
Bi1 - O43	2.400(4)	C1 - C2	1.501(8)
Bi1 - O5	2.653(5)	C2 - C3	1.368(8)
Bi1 - O7	2.198(4)	C2 - C7	1.398(7)
Bi1 - O71	2.203(4)	C3 - C4	1.385(9)
F1 - C3	1.358(7)	C4 - C5	1.367(9)
F2 - C4	1.323(7)	C5 - C6	1.370(9)
F3 - C5	1.339(8)	C6 - C7	1.380(8)
F4 - C6	1.349(7)	C7 - C8	1.494(8)

$$^11\text{-X},1\text{-Y},\text{-Z}; ^21\text{-X},1\text{-Y},1\text{-Z}; ^31\text{-X},-1/2+\text{Y},1/2\text{-Z}$$

Table S6 Bond Angles [°] for [BiO(TFPHA)H₂O]·H₂O

O1-Bi1-Bi11	78.16(10)	C1-O2-Bi12	119.3(3)
O1-Bi1-O22	91.25(14)	C8-O3-Bi14	86.3(3)
O1-Bi1-O33	142.79(14)	C8-O4-Bi14	99.5(3)
O1-Bi1-O5	74.06(15)	Bi1-O7-Bi11	111.70(17)
O22-Bi1-Bi11	107.19(9)	O1-C1-O2	124.2(5)
O22-Bi1-O33	125.48(13)	O1-C1-C2	117.2(5)
O22-Bi1-O5	138.02(14)	O2-C1-C2	118.5(5)
O33-Bi1-Bi11	94.27(10)	C3-C2-C1	118.2(5)
O43-Bi1-Bi11	86.77(10)	C3-C2-C7	119.1(6)
O43-Bi1-O1	159.84(15)	C7-C2-C1	122.7(5)
O43-Bi1-O22	80.41(13)	F1-C3-C2	120.7(6)
O43-Bi1-O33	50.81(13)	F1-C3-C4	117.1(6)
O43-Bi1-O5	123.93(15)	C2-C3-C4	122.2(6)
O5-Bi1-Bi11	107.78(11)	F2-C4-C3	120.7(6)
O5-Bi1-O33	73.84(15)	F2-C4-C5	120.8(6)
O71-Bi1-Bi11	34.11(10)	C5-C4-C3	118.5(6)
O7-Bi1-Bi11	34.19(11)	F3-C5-C4	119.6(6)
O71-Bi1-O1	80.60(15)	F3-C5-C6	120.3(7)
O7-Bi1-O1	79.84(15)	C4-C5-C6	120.1(6)
O7-Bi1-O22	73.01(14)	F4-C6-C5	116.9(6)
O71-Bi1-O22	141.28(13)	F4-C6-C7	121.1(5)
O71-Bi1-O33	73.80(14)	C5-C6-C7	122.0(6)
O7-Bi1-O33	113.76(15)	C2-C7-C8	119.8(5)
O7-Bi1-O43	80.18(15)	C6-C7-C2	118.1(5)
O71-Bi1-O43	94.42(16)	C6-C7-C8	122.1(5)
O7-Bi1-O5	138.51(16)	O3-C8-O4	122.8(5)
O71-Bi1-O5	75.96(15)	O3-C8-C7	117.6(5)
O7-Bi1-O71	68.30(17)	O4-C8-C7	119.6(5)
C1-O1-Bi1	109.3(4)	-	-
$^11\text{-X},1\text{-Y},\text{-Z}; ^21\text{-X},1\text{-Y},1\text{-Z}; ^31\text{-X},-1/2+\text{Y},1/2\text{-Z}; ^41\text{-X},1/2+\text{Y},1/2\text{-Z}$			

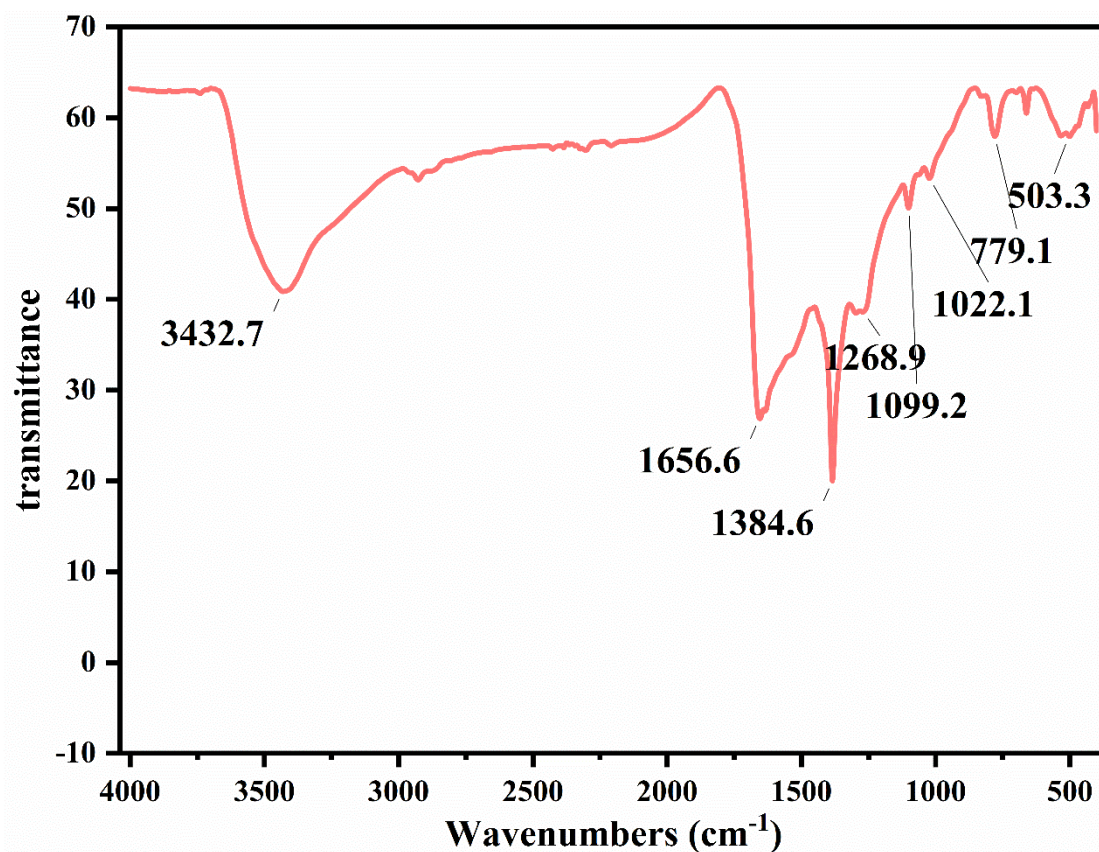


Fig. S3 FTIR spectra of $[\text{Bi}_2(\text{DHBQDC})(\text{OX})_2(\text{DMF})_6]$

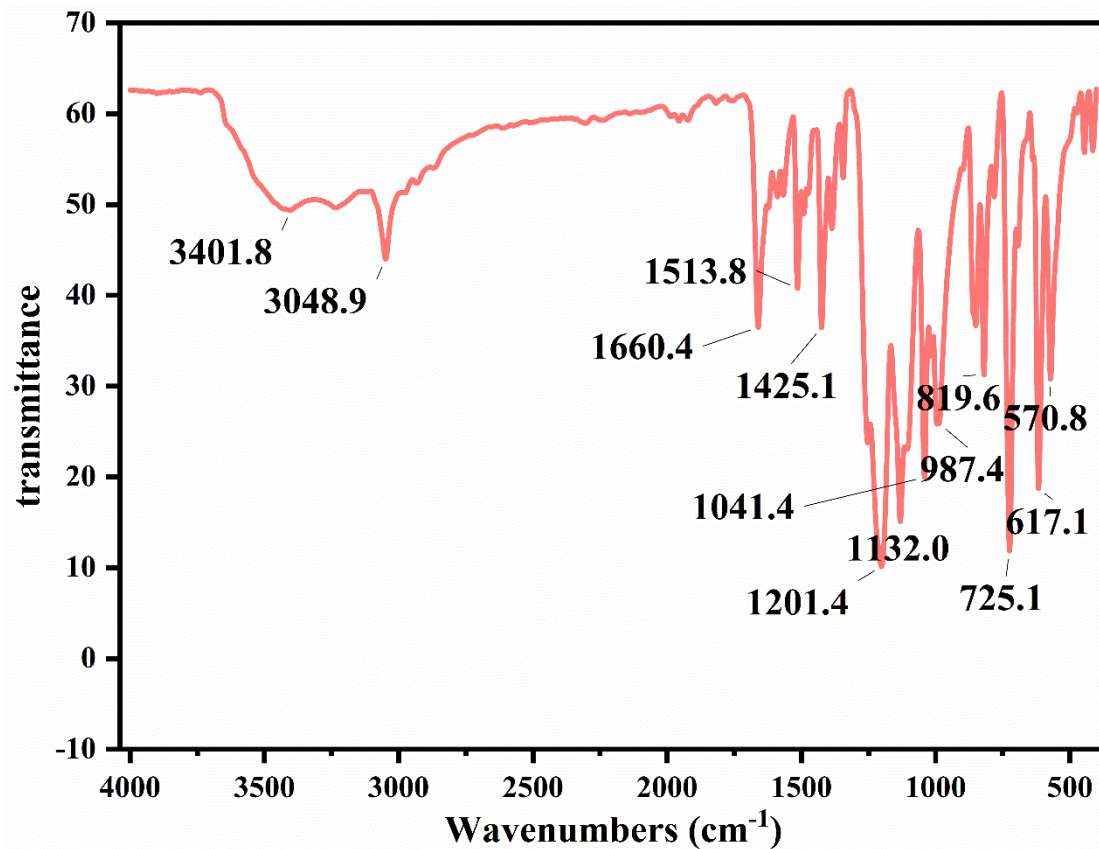


Fig. S4 FTIR spectra of $[\text{Bi}(\text{BPSA})(\text{PHON})(\text{Ph})] \cdot 3\text{DMF}$

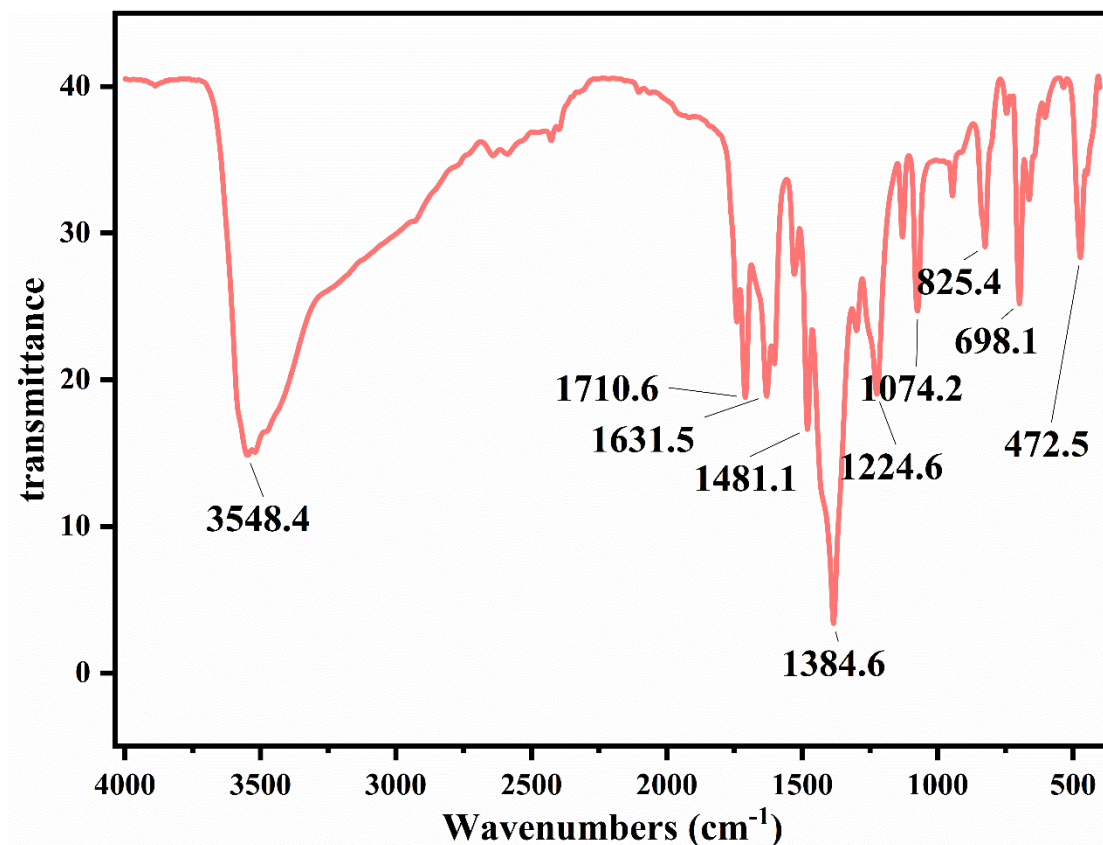


Fig. S5 FTIR spectra of $[\text{BiO}(\text{TFPHA})\text{H}_2\text{O}] \cdot \text{H}_2\text{O}$

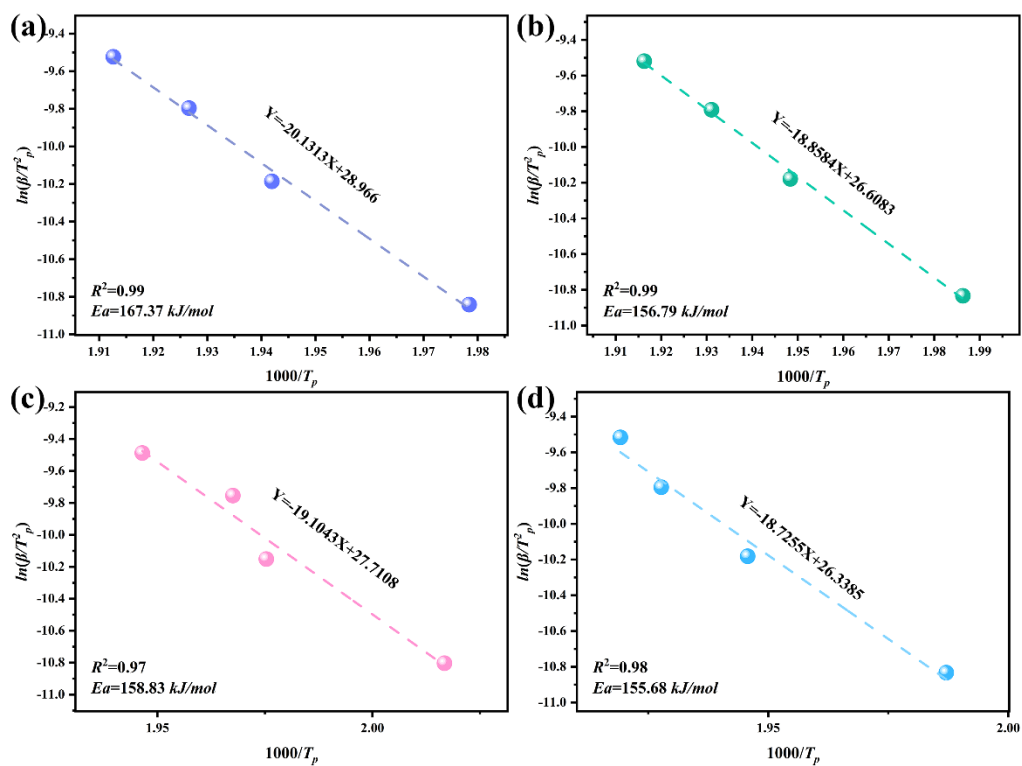


Fig. S5 fitting curves of RDX (a); RDX + Cat. 1 (b); RDX + Cat. 2 (c); RDX + Cat. 3 (d)