

Supplementary information

Halogen regulation of multifunctional hybrid materials with photoluminescence and dielectric response

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Experimental Section

Synthesis and Growth of Crystals

All chemical reagents used in this work were obtained from commercial sources without further purification. The synthesis of the ligands 2,5-FBTA can refer to previous reports. Weigh 2 mmol 2,5-FBTA in a beaker, dissolve it with 15 mL methanol solution, then add hydrobromic acid, and then add 2 mmol MnBr₂. After complete dissolution, it slowly evaporates at room temperature, and after a few weeks, a green FBTAM-Br massive crystal is obtained. The crystals of FBTAM-Cl and FBTAM-I were obtained by the same method.

Detailed methods of measurements

Variable-Temperature Single-crystal XRD

The Rigaku Saturn 724 diffractometer with Mo K α radiation ($\lambda = 0.71073 \text{ \AA}$) was used to obtain single crystal X-ray diffraction data. The direct method was used to solve the variable temperature crystal structure data, and the SHELXL software was used to analyze and refine the crystal structure. Import the generated CIF file into DIAMOND to draw the corresponding asymmetric cell diagram and stack diagram, and calculate the selected bond distances and angles through Mercury. Table S1-S8 summarize the data collection of these crystals. These X-ray crystal structures have been stored at the Cambridge Crystallography Data Center (storage number CCDC 2368921-2368925) and are available free of charge from CCDC at www.ccdc.cam.ac.uk/getstructures.

DSC Measurement

Grind crystal into powder, weigh about 10 mg of powder, and place it in an aluminum crucible. Under nitrogen protection of the environment, the NETZSCH DSC 214 Polymer instrument is used to uniformly heat and cool at a rate of 20 K/min.

Dielectric Measurement

Press the powder sample into sheets, use conductive silver glue and copper wire as the medium, and connect the sheet sample to both ends of the electrode to make a capacitor. The complex dielectric constant at different frequencies was measured using Tonghui TH2828A instrument at 1V AC voltage.

Powder X-ray diffraction

Powder X-ray diffraction (PXRD) measurements were performed at room temperature on a Rigaku SmartLab SE X-ray diffractometer. The diffraction pattern is recorded at 2θ between 0-50° within the range, the step size is 0.01°. Variable temperature powder X-ray diffraction pattern tested in the temperature range of 298-433 K through programmed heating and cooling.

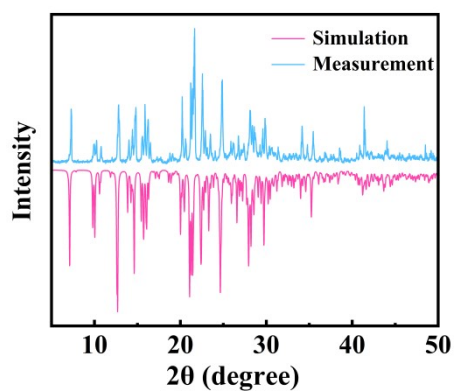


Fig. S1 PXRd spectra of FBTAM-Br at LTP.

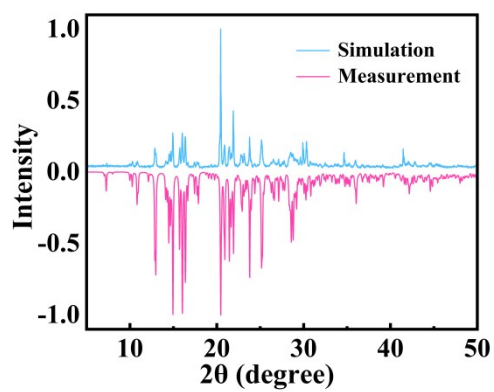


Fig. S2 PXRd spectra of FBTAM-Cl at LTP.

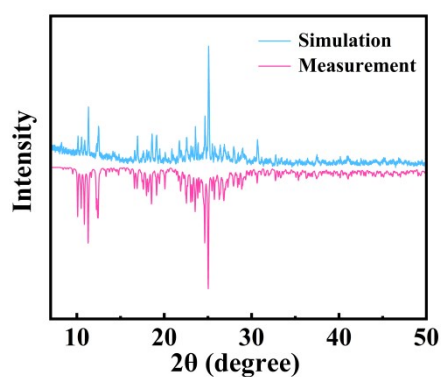


Fig. S3 PXRd spectra of FBTAM-I at LTP.

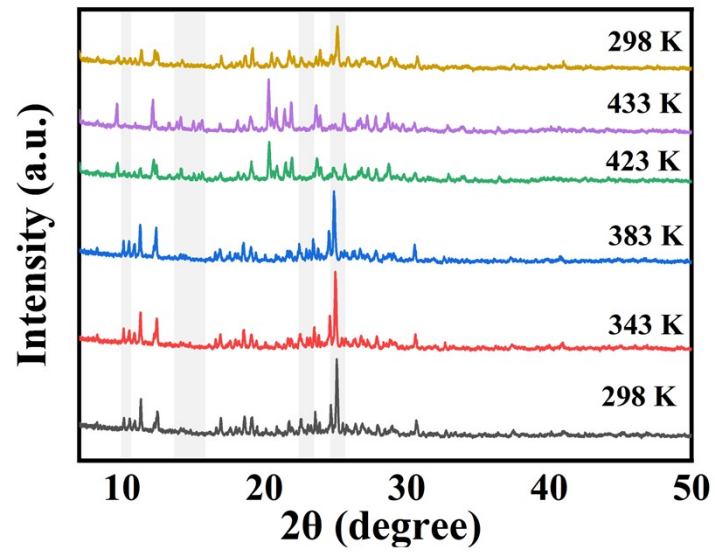


Fig. S4 Variable-temperature PXRD spectra of FBTAM-I.

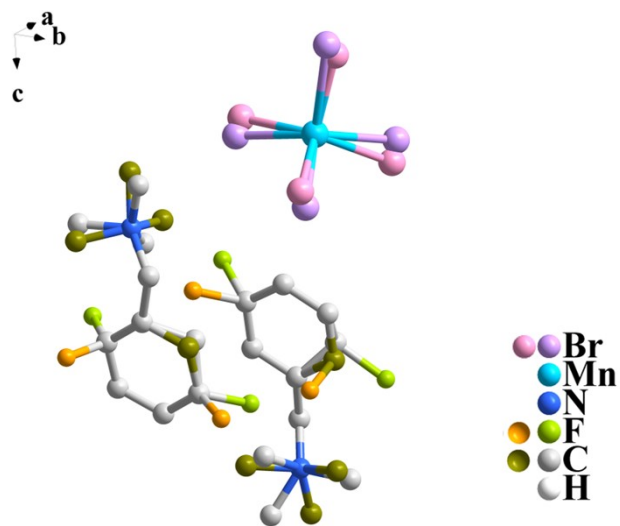


Fig. S5 The crystal structure of FBTAM-Br in the HTP.

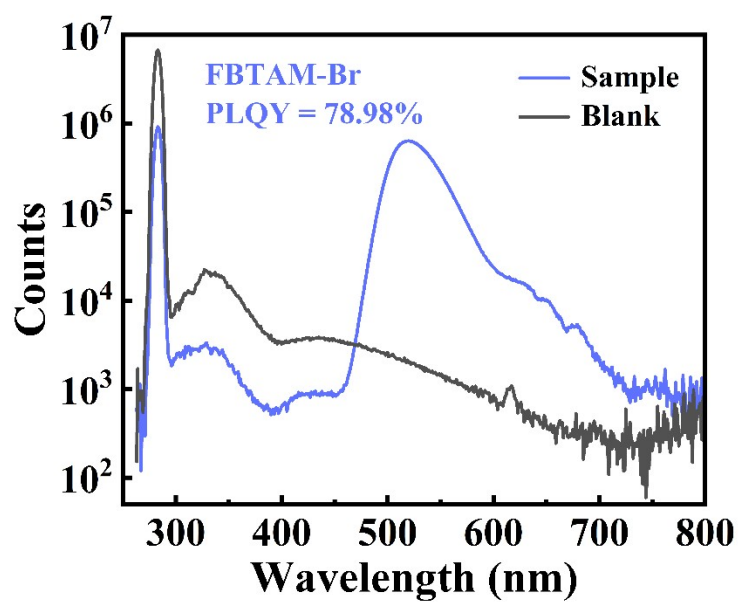


Fig. S6 Quantum yield of FBTAM-Br.

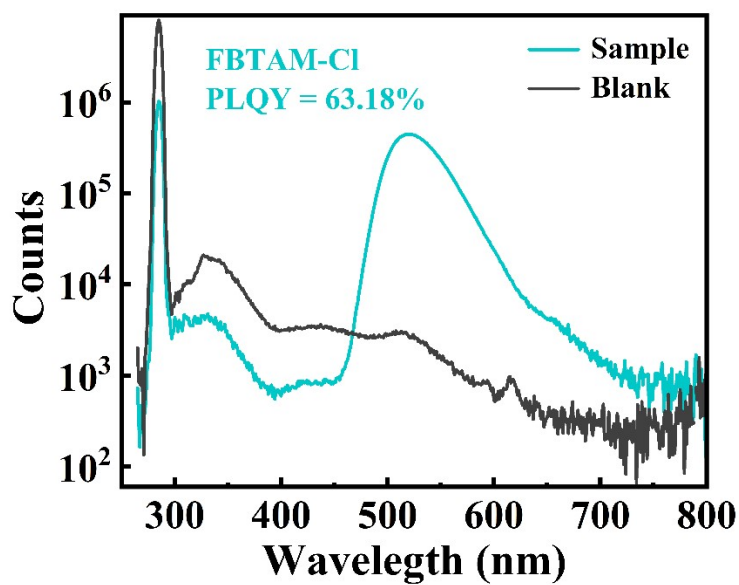


Fig. S7 Quantum yield of FBTAM-Cl.

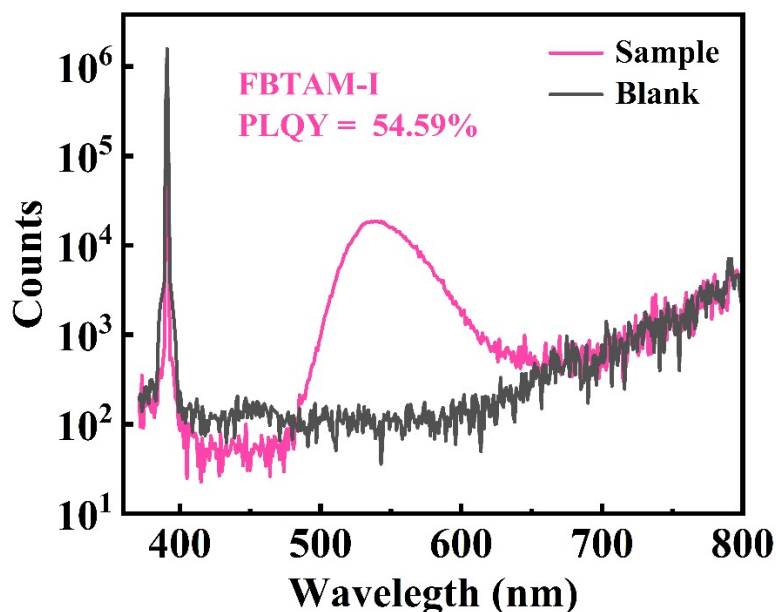


Fig. S8 Quantum yield of FBTAM-I.

Table S1 Crystal data and structure refinements for FBTAM-Br in the LTP and HTP.

	FBTAM-Br (300K)	FBTAM-Br (443K)
Empirical formula	C ₂₀ H ₂₈ Br ₄ F ₄ MnN ₂	C ₂₀ H ₂₈ Br ₄ F ₄ MnN ₂
Formula weight	747.02	747.02
Space group	<i>P</i> 2 ₁ / <i>c</i> (14)	<i>P</i> 2 ₁ / <i>n</i> (14)
Crystal system	monoclinic	monoclinic
a/ Å	27.665(9)	9.0041(19)
b/ Å	8.864(3)	13.0052(15)
c/ Å	25.542(4)	24.957(4)
α/°	90	90
β/°	116.083(13)	90.039(11)
γ/°	90	90
Volume/ Å³	5626(3)	2922.4(8)
Z	8	4
F(000)	2904	1452
GOF	1.137	1.094
R_{int}	0.1243	0.1328
R₁	0.1093	0.1137
wR₂	0.3092	0.2658

Table S2 The bond lengths (Å) and angles (°) of FBTAM-Br in the LTP.

Atom–Atom	Length [Å]	Atom–Atom–Atom	Angle [°]
Br1–Mn1	2.4868(15)	Br1–Mn1–Br2	111.09(5)
Br4–Mn2	2.5024(16)	Br1–Mn1–Br3	112.52(6)
Br6–Mn2	2.5011(17)	Br1–Mn1–Br7	108.43(5)
Br8–Mn2	2.5117(16)	Br3–Mn1–Br2	108.48(6)
Br2–Mn1	2.5107(17)	Br7–Mn1–Br2	110.45(6)
Br5–Mn2	2.4879(16)	Br7–Mn1–Br3	105.74(5)
Br3–Mn1	2.5041(15)	Br4–Mn2–Br8	107.52(5)
Br7–Mn1	2.5015(17)	Br6–Mn2–Br4	106.86(6)
N1–C4	1.499(10)	Br6–Mn2–Br8	107.59(6)

N1-C12	1.503(13)	Br5-Mn2-Br4	109.29(6)
N1-C40	1.463(14)	Br5-Mn2-Br6	113.51(5)
N1-C2	1.486(13)	Br5-Mn2-Br8	111.78(6)
F1-C20	1.294(14)	C4-N1-C12	107.4(7)
N4-C16	1.554(11)	C40-N1-C4	111.2(8)
N4-C34	1.472(12)	C40-N1-C12	110.1(8)
N4-C36	1.486(12)	C40-N1-C2	109.1(9)
N4-C44	1.498(11)	C2-N1-C4	110.6(6)
F4-C23	1.363(10)	C2-N1-C12	108.4(9)
N2-C8	1.534(11)	C34-N4-C16	109.7(6)
N2-C22	1.494(12)	C34-N4-C36	111.2(8)
N2-C15	1.475(12)	C34-N4-C44	110.6(8)
N2-C37	1.466(10)	C36-N4-C16	111.3(7)
F6-C19	1.305(13)	C36-N4-C44	106.8(7)
N3-C28	1.489(12)	C44-N4-C16	107.1(7)
N3-C38	1.473(15)	C22-N2-C8	111.0(7)
N3-C42	1.480(13)	C15-N2-C8	111.3(7)
N3-C7	1.522(11)	C15-N2-C22	109.5(7)
C1-C6	1.397(13)	C37-N2-C8	107.7(7)
C1-C16	1.502(10)	C37-N2-C22	110.7(7)
C1-C20	1.353(11)	C37-N2-C15	106.5(8)
C4-H4A	0.9700	C28-N3-C7	105.5(8)
C4-H4B	0.9700	C38-N3-C28	109.9(9)
C4-C14	1.500(12)	C38-N3-C42	110.6(8)
F8-C31	1.363(8)	C38-N3-C7	111.1(7)
C6-H6	0.9300	C42-N3-C28	108.6(7)
C6-C23	1.385(9)	C42-N3-C7	110.9(8)
C8-H8A	0.9700	C6-C1-C16	119.9(7)
C8-H8B	0.9700	C20-C1-C6	119.0(8)
C8-C26	1.499(8)	C20-C1-C16	120.9(9)
C10-F12	1.364(10)	N1-C4-H4A	108.1
C10-C24	1.399(13)	N1-C4-H4B	108.1
C10-C9	1.397(10)	N1-C4-C14	116.8(8)
C10-F9	1.376(8)	H4A-C4-H4B	107.3
C10-C21	1.400(9)	C14-C4-H4A	108.1
F10-C35	1.360(11)	C14-C4-H4B	108.1
C12-H12A	0.9600	C1-C6-H6	120.1
C12-H12B	0.9600	C23-C6-C1	119.8(7)
C12-H12C	0.9600	C23-C6-H6	120.1
C14-C24	1.345(14)	N2-C8-H8A	108.7
C14-C31	1.377(12)	N2-C8-H8B	108.7
C16-H16A	0.9700	H8A-C8-H8B	107.6
C16-H16B	0.9700	C26-C8-N2	114.2(6)
C18-H18	0.9300	C26-C8-H8A	108.7
C18-C3	1.32(2)	C26-C8-H8B	108.7
C18-C19	1.438(13)	F12-C10-C24	120.5(10)
C20-C39	1.388(16)	F12-C10-C9	115.6(10)
C22-H22A	0.9600	C24-C10-C21	116.2(7)
C22-H22B	0.9600	C9-C10-C24	123.7(8)
C22-H22C	0.9600	F9-C10-C24	113.0(9)
C24-H24	0.9300	F9-C10-C21	130.7(9)
C26-C13	1.406(10)	N1-C12-H12A	109.5
C26-C35	1.335(9)	N1-C12-H12B	109.5
C26-C11	1.404(10)	N1-C12-H12C	109.5
C28-H28A	0.9600	H12A-C12-H12B	109.5
C28-H28B	0.9600	H12A-C12-H12C	109.5
C28-H28C	0.9600	H12B-C12-H12C	109.5

C30-H30	0.9300	C24-C14-C4	121.9(10)
C30-C23	1.302(14)	C24-C14-C31	117.6(9)
C30-C39	1.46(2)	C31-C14-C4	120.2(7)
C32-H32	0.9300	N4-C16-H16A	108.3
C32-C45	1.308(14)	N4-C16-H16B	108.3
C32-C17	1.425(15)	C1-C16-N4	115.9(7)
F14-C27	1.371(10)	C1-C16-H16A	108.3
C34-H34A	0.9600	C1-C16-H16B	108.3
C34-H34B	0.9600	H16A-C16-H16B	107.4
C34-H34C	0.9600	C3-C18-H18	120.5
C36-H36A	0.9600	C3-C18-C19	118.9(13)
C36-H36B	0.9600	C19-C18-H18	120.5
C36-H36C	0.9600	F1-C20-C1	121.0(9)
C38-H38A	0.9600	F1-C20-C39	117.9(9)
C38-H38B	0.9600	C1-C20-C39	121.1(11)
C38-H38C	0.9600	N2-C22-H22A	109.5
C40-H40A	0.9600	N2-C22-H22B	109.5
C40-H40B	0.9600	N2-C22-H22C	109.5
C40-H40C	0.9600	H22A-C22-H22B	109.5
C42-H42A	0.9600	H22A-C22-H22C	109.5
C42-H42B	0.9600	H22B-C22-H22C	109.5
C42-H42C	0.9600	C10-C24-H24	119.4
C44-H44A	0.9600	C14-C24-C10	121.2(11)
C44-H44B	0.9600	C14-C24-H24	119.4
C44-H44C	0.9600	C13-C26-C8	114.3(6)
C45-C7	1.517(11)	C35-C26-C8	125.2(7)
C45-C19	1.346(15)	C35-C26-C13	120.2(6)
C23-F11	1.362(10)	C35-C26-C11	116.4(6)
C3-H3	0.9300	C11-C26-C8	118.1(6)
C3-C17	1.34(2)	N3-C28-H28A	109.5
F7-C17	1.367(9)	N3-C28-H28B	109.5
C25-H25	0.9300	N3-C28-H28C	109.5
C25-C27	1.408(9)	H28A-C28-H28B	109.5
C25-C33	1.407(10)	H28A-C28-H28C	109.5
C13-H13	0.9300	H28B-C28-H28C	109.5
C13-C27	1.403(8)	C23-C30-H30	120.8
C7-H7A	0.9700	C23-C30-C39	118.5(10)
C7-H7B	0.9700	C39-C30-H30	120.8
C29-H29	0.9300	C45-C32-H32	120.1
C29-C31	1.404(8)	C45-C32-C17	119.7(12)
C29-C9	1.399(10)	C17-C32-H32	120.1
C15-H15A	0.9600	N4-C34-H34A	109.5
C15-H15B	0.9600	N4-C34-H34B	109.5
C15-H15C	0.9600	N4-C34-H34C	109.5
C31-F2	1.365(9)	H34A-C34-H34B	109.5
C31-C43	1.400(9)	H34A-C34-H34C	109.5
C2-H2A	0.9600	H34B-C34-H34C	109.5
C2-H2B	0.9600	N4-C36-H36A	109.5
C2-H2C	0.9600	N4-C36-H36B	109.5
C33-H33A	0.9300	N4-C36-H36C	109.5
C33-H33	0.9300	H36A-C36-H36B	109.5
C33-C35	1.401(9)	H36A-C36-H36C	109.5
C33-C5	1.394(10)	H36B-C36-H36C	109.5
C17-F5	1.365(10)	N3-C38-H38A	109.5
C35-F3	1.367(10)	N3-C38-H38B	109.5
C9-H9	0.9300	N3-C38-H38C	109.5
C37-H37A	0.9600	H38A-C38-H38B	109.5

C37-H37B	0.9600	H38A-C38-H38C	109.5
C37-H37C	0.9600	H38B-C38-H38C	109.5
C39-H39	0.9300	N1-C40-H40A	109.5
F13-C41	1.364(11)	N1-C40-H40B	109.5
C5-H5	0.9300	N1-C40-H40C	109.5
C5-C41	1.396(9)	H40A-C40-H40B	109.5
C41-C11	1.402(8)	H40A-C40-H40C	109.5
C21-H21	0.9300	H40B-C40-H40C	109.5
C21-C43	1.399(10)	N3-C42-H42A	109.5
C43-H43	0.9300	N3-C42-H42B	109.5
C11-H11	0.9300	N3-C42-H42C	109.5
		H42A-C42-H42B	109.5
		H42A-C42-H42C	109.5
		H42B-C42-H42C	109.5
		N4-C44-H44A	109.5
		N4-C44-H44B	109.5
		N4-C44-H44C	109.5
		H44A-C44-H44B	109.5
		H44A-C44-H44C	109.5
		H44B-C44-H44C	109.5
		C32-C45-C7	120.6(10)
		C32-C45-C19	121.2(9)
		C19-C45-C7	118.1(8)
		F4-C23-C6	108.8(6)
		C30-C23-F4	128.3(8)
		C30-C23-C6	122.8(9)
		C30-C23-F11	111.3(8)
		F11-C23-C6	124.8(7)
		C18-C3-H3	119.5
		C18-C3-C17	121.0(11)
		C17-C3-H3	119.5
		C27-C25-H25	114.4
		C33-C25-H25	114.4
		C33-C25-C27	131.3(8)
		C26-C13-H13	118.3
		C27-C13-C26	123.4(8)
		C27-C13-H13	118.3
		F14-C27-C25	130.2(7)
		F14-C27-C13	120.0(7)
		C13-C27-C25	109.5(8)
		N3-C7-H7A	108.4
		N3-C7-H7B	108.4
		C45-C7-N3	115.4(8)
		C45-C7-H7A	108.4
		C45-C7-H7B	108.4
		H7A-C7-H7B	107.5
		C31-C29-H29	118.0
		C9-C29-H29	118.0
		C9-C29-C31	124.0(9)
		N2-C15-H15A	109.5
		N2-C15-H15B	109.5
		N2-C15-H15C	109.5
		H15A-C15-H15B	109.5
		H15A-C15-H15C	109.5
		H15B-C15-H15C	109.5
		F8-C31-C14	120.6(7)
		F8-C31-C29	118.3(9)

C14-C31-C29	120.1(7)
C14-C31-C43	124.0(7)
F2-C31-C14	115.9(8)
F2-C31-C43	120.0(9)
N1-C2-H2A	109.5
N1-C2-H2B	109.5
N1-C2-H2C	109.5
H2A-C2-H2B	109.5
H2A-C2-H2C	109.5
H2B-C2-H2C	109.5
C25-C33-H33A	124.8
C35-C33-C25	110.4(7)
C35-C33-H33A	124.8
C35-C33-H33	116.9
C5-C33-H33	116.9
C5-C33-C35	126.2(7)
C3-C17-C32	119.6(9)
C3-C17-F7	124.8(11)
C3-C17-F5	117.6(12)
F7-C17-C32	112.4(12)
F5-C17-C32	120.8(13)
F10-C35-C33	111.1(7)
C26-C35-F10	124.0(7)
C26-C35-C33	124.0(7)
C26-C35-F3	113.9(6)
F3-C35-C33	121.6(7)
C10-C9-C29	111.9(7)
C10-C9-H9	124.1
C29-C9-H9	124.1
N2-C37-H37A	109.5
N2-C37-H37B	109.5
N2-C37-H37C	109.5
H37A-C37-H37B	109.5
H37A-C37-H37C	109.5
H37B-C37-H37C	109.5
F6-C19-C18	116.6(11)
F6-C19-C45	123.9(8)
C45-C19-C18	119.4(10)
C20-C39-C30	118.6(10)
C20-C39-H39	120.7
C30-C39-H39	120.7
C33-C5-H5	128.6
C33-C5-C41	102.9(7)
C41-C5-H5	128.6
F13-C41-C5	105.1(7)
F13-C41-C11	119.2(8)
C5-C41-C11	135.1(9)
C10-C21-H21	118.6
C43-C21-C10	122.7(9)
C43-C21-H21	118.6
C31-C43-H43	123.5
C21-C43-C31	113.0(9)
C21-C43-H43	123.5
C26-C11-H11	123.2
C41-C11-C26	113.6(8)
C41-C11-H11	123.2

Table S3 The bond lengths (Å) and angles (°) of FBTAM-Br in the HTP.

Atom-Atom	Length [Å]	Atom-Atom-Atom	Angle [°]
Br1B-Mn1	2.48(2)	Br1B-Mn1-Br4B	105.1(9)
Br4B-Mn1	2.74(2)	Br1B-Mn1-Br2B	118.4(12)
Br2B-Mn1	2.56(3)	Br1B-Mn1-Br3B	110.1(10)
Br3B-Mn1	2.49(3)	Br2B-Mn1-Br4B	95.1(13)
Mn1-Br2A	2.466(16)	Br3B-Mn1-Br4B	103.5(10)
Mn1-Br1A	2.513(10)	Br3B-Mn1-Br2B	120.6(11)
Mn1-Br4A	2.357(18)	Br2A-Mn1-Br1A	105.8(6)
Mn1-Br3A	2.512(16)	Br2A-Mn1-Br3A	101.0(9)
N1-C1	1.56(7)	Br4A-Mn1-Br2A	114.7(9)
N1-C4	1.40(3)	Br4A-Mn1-Br1A	116.4(6)
N1-C6	1.497(10)	Br4A-Mn1-Br3A	107.9(4)
N1-C8	1.495(10)	Br3A-Mn1-Br1A	110.0(5)
N1-C24	1.42(5)	C4-N1-C1	112(3)
N1-C26	1.480(18)	C4-N1-C6	119(2)
N1-C28	1.63(5)	C4-N1-C8	94(2)
C1-H1A	0.9604	C4-N1-C24	110(3)
C1-H1B	0.9598	C4-N1-C26	132(2)
C1-H1C	0.9594	C4-N1-C28	97.7(19)
C4-H4A	0.9700	C6-N1-C1	109(3)
C4-H4B	0.9700	C8-N1-C1	109(4)
C4-C18	1.521(10)	C8-N1-C6	114(2)
C6-H6A	0.9600	C24-N1-C26	112(3)
C6-H6B	0.9602	C24-N1-C28	106(3)
C6-H6C	0.9599	C26-N1-C28	91(2)
C8-H8A	0.9600	N1-C1-H1A	115.8
C8-H8B	0.9598	N1-C1-H1B	106.8
C8-H8C	0.9599	N1-C1-H1C	105.6
F1-C10	1.59(2)	H1A-C1-H1B	109.5
C10-C12	1.3900	H1A-C1-H1C	109.5
C10-C20	1.3900	H1B-C1-H1C	109.5
C10-F6	1.59(2)	N1-C4-H4A	109.2
C12-H12	0.9300	N1-C4-H4B	109.2
C12-C14	1.3900	N1-C4-C18	112(2)
C14-H14A	0.9300	H4A-C4-H4B	107.9
C14-H14	0.9300	C18-C4-H4A	109.2
C14-C16	1.3900	C18-C4-H4B	109.2
C14-C22	1.410(17)	N1-C6-H6A	107.0
C16-C18	1.3900	N1-C6-H6B	107.3
C16-F8	1.62(2)	N1-C6-H6C	114.0
C18-C20	1.3900	H6A-C6-H6B	109.5
C18-C22	1.411(17)	H6A-C6-H6C	109.5
C20-H20	0.9300	H6B-C6-H6C	109.4
F4-C22	1.61(2)	N1-C8-H8A	108.4
C24-H24A	0.9600	N1-C8-H8B	108.7
C24-H24B	0.9600	N1-C8-H8C	111.2
C24-H24C	0.9600	H8A-C8-H8B	109.5
C26-H26A	0.9600	H8A-C8-H8C	109.5
C26-H26B	0.9601	H8B-C8-H8C	109.5
C26-H26C	0.9598	C12-C10-F1	104(2)
C28-H28A	0.9598	C12-C10-C20	120.0
C28-H28B	0.9597	C12-C10-F6	116.4(18)
C28-H28C	0.9599	C20-C10-F1	119(2)
C7-H7	0.9300	C20-C10-F6	109.7(18)
C7-C15	1.3900	C10-C12-H12	120.0
C7-C19	1.3900	C10-C12-C14	120.0

C15-H15	0.9300	C14-C12-H12	120.0
C15-C2	1.3900	C12-C14-H14A	120.0
C2-C17	1.3900	C12-C14-H14	126.5
C2-F3	1.58(2)	C12-C14-C16	120.0
C2-F7	1.55(2)	C12-C14-C22	107.0(17)
C17-C9	1.3900	C16-C14-H14A	120.0
C17-C11	1.611(18)	C22-C14-H14	126.5
C17-C3	1.45(9)	C14-C16-C18	120.0
C9-H9	0.9300	C14-C16-F8	89.9(18)
C9-C19	1.3900	C18-C16-F8	93.6(19)
C19-F2	1.474(15)	C16-C18-C4	129.5(17)
C19-C3	1.410(15)	C20-C18-C4	109.0(17)
C19-F5	1.546(19)	C20-C18-C16	120.0
C5-H5A	0.9603	C20-C18-C22	107.0(17)
C5-H5B	0.9600	C22-C18-C4	127(2)
C5-H5C	0.9599	C10-C20-H20	120.0
C5-N2	1.482(13)	C18-C20-C10	120.0
N2-C21	1.481(13)	C18-C20-H20	120.0
N2-C11	1.535(17)	C14-C22-C18	117.2(18)
N2-C23	1.479(13)	C14-C22-F4	115(3)
N2-C25	1.453(16)	C18-C22-F4	102(2)
N2-C13	1.455(16)	N1-C24-H24A	109.5
N2-C27	1.453(16)	N1-C24-H24B	109.5
C21-H21A	0.9600	N1-C24-H24C	109.5
C21-H21B	0.9597	H24A-C24-H24B	109.5
C21-H21C	0.9597	H24A-C24-H24C	109.5
C11-H11A	0.9700	H24B-C24-H24C	109.5
C11-H11B	0.9700	N1-C26-H26A	137.3
C23-H23A	0.9600	N1-C26-H26B	81.9
C23-H23B	0.9600	N1-C26-H26C	104.4
C23-H23C	0.9599	H26A-C26-H26B	109.5
C3-H3	0.9300	H26A-C26-H26C	109.5
C25-H25A	0.9602	H26B-C26-H26C	109.5
C25-H25B	0.9602	N1-C28-H28A	111.8
C25-H25C	0.9596	N1-C28-H28B	92.1
C13-H13A	0.9598	N1-C28-H28C	122.8
C13-H13B	0.9597	H28A-C28-H28B	109.5
C13-H13C	0.9601	H28A-C28-H28C	109.5
C27-H27A	0.9603	H28B-C28-H28C	109.4
C27-H27B	0.9597	C15-C7-H7	120.0
C27-H27C	0.9602	C15-C7-C19	120.0
		C19-C7-H7	120.0
		C7-C15-H15	120.0
		C2-C15-C7	120.0
		C2-C15-H15	120.0
		C15-C2-F3	90(2)
		C15-C2-F7	104(2)
		C17-C2-C15	120.0
		C17-C2-F3	124(3)
		C17-C2-F7	95.6(19)
		C2-C17-C9	120.0
		C2-C17-C11	142(2)
		C2-C17-C3	114.9(18)
		C9-C17-C11	98(2)
		C3-C17-C11	102(3)
		C17-C9-H9	120.0
		C17-C9-C19	120.0

C19-C9-H9	120.0
C7-C19-F2	128(2)
C7-C19-C3	116(2)
C7-C19-F5	101.3(18)
C9-C19-C7	120.0
C9-C19-F5	123(2)
C3-C19-F2	109(2)
H5A-C5-H5B	109.5
H5A-C5-H5C	109.5
H5B-C5-H5C	109.5
N2-C5-H5A	119.7
N2-C5-H5B	107.6
N2-C5-H5C	100.6
C5-N2-C11	94.6(19)
C21-N2-C5	101(5)
C21-N2-C11	100(2)
C23-N2-C5	102(2)
C23-N2-C21	95(4)
C23-N2-C11	155(4)
C25-N2-C11	120(3)
C25-N2-C13	106(2)
C25-N2-C27	105(2)
C13-N2-C11	106(3)
C27-N2-C11	110(2)
C27-N2-C13	110(3)
N2-C21-H21A	108.9
N2-C21-H21B	117.8
N2-C21-H21C	101.3
H21A-C21-H21B	109.5
H21A-C21-H21C	109.5
H21B-C21-H21C	109.5
C17-C11-H11A	110.9
C17-C11-H11B	110.9
N2-C11-C17	104.3(17)
N2-C11-H11A	110.9
N2-C11-H11B	110.9
H11A-C11-H11B	108.9
N2-C23-H23A	107.2
N2-C23-H23B	108.7
N2-C23-H23C	112.5
H23A-C23-H23B	109.5
H23A-C23-H23C	109.5
H23B-C23-H23C	109.5
C17-C3-H3	122.7
C19-C3-C17	115(5)
C19-C3-H3	122.7
N2-C25-H25A	111.5
N2-C25-H25B	125.9
N2-C25-H25C	88.4
H25A-C25-H25B	109.5
H25A-C25-H25C	109.4
H25B-C25-H25C	109.5
N2-C13-H13A	91.5
N2-C13-H13B	119.2
N2-C13-H13C	115.9
H13A-C13-H13B	109.5
H13A-C13-H13C	109.5

H13B–C13–H13C	109.5
N2–C27–H27A	96.8
N2–C27–H27B	96.0
N2–C27–H27C	133.6
H27A–C27–H27B	109.5
H27A–C27–H27C	109.4
H27B–C27–H27C	109.5

Table S4 Crystal data and structure refinements for FBTAM-Cl in the LTP and HTP.

	FBTAM-Cl (302K)	FBTAM-Cl (433K)
Empirical formula	C ₄₀ Cl ₈ F ₈ Mn ₂ N ₄	C ₂₀ H ₂₈ Cl ₄ F ₄ MnN ₂
Formula weight	1081.92	569.18
Space group	<i>P</i> 2 ₁ / <i>c</i> (14)	<i>P</i> 2 ₁ 2 ₁ 2 ₁ (19)
Crystal system	monoclinic	orthorhombic
a/ Å	27.063(2)	8.8604(13)
b/ Å	8.6781(3)	12.787(3)
c/ Å	25.104(2)	24.679(5)
α/°	90	90
β/°	116.085(10)	90
γ/°	90	90
Volume/ Å³	5295.4(8)	2796.1(9)
Z	4	4
F(000)	2104	1164
GOF	1.040	1.038
R_{int}	0.1034	0.0736
R₁	0.1132	0.1054
wR₂	0.3012	0.2839

Table S5 The bond lengths (Å) and angles (°) of FBTAM-Cl in the LTP.

Atom–Atom	Length [Å]	Atom–Atom–Atom	Angle [°]
Mn01–Cl10	2.439(2)	Cl05–Mn01–Cl10	112.07(8)
Mn01–Cl05	2.426(2)	Cl06–Mn01–Cl10	113.29(9)
Mn01–Cl06	2.390(2)	Cl06–Mn01–Cl05	107.40(8)
Mn01–Cl08	2.382(2)	Cl08–Mn01–Cl10	108.67(8)
Mn02–Cl04	2.447(2)	Cl08–Mn01–Cl05	107.08(9)
Mn02–Cl07	2.388(2)	Cl08–Mn01–Cl06	108.08(9)
Mn02–Cl09	2.396(2)	Cl07–Mn02–Cl04	110.62(8)
Mn02–Cl0A	2.387(2)	Cl07–Mn02–Cl09	108.43(8)
N00B–C00S	1.520(11)	Cl09–Mn02–Cl04	110.42(9)
N00B–C012	1.476(11)	Cl0A–Mn02–Cl04	108.59(8)
N00B–C01F	1.507(13)	Cl0A–Mn02–Cl07	112.91(10)
N00B–C01M	1.483(14)	Cl0A–Mn02–Cl09	105.77(11)
N00C–C00Q	1.536(11)	C012–N00B–C00S	111.4(7)
N00C–C010	1.468(12)	C012–N00B–C01F	108.3(9)
N00C–C015	1.521(12)	C012–N00B–C01M	109.9(9)
N00C–C017	1.507(13)	C01F–N00B–C00S	106.0(7)
F00D–C00V	1.362(12)	C01M–N00B–C00S	111.6(8)
N00E–C00R	1.529(11)	C01M–N00B–C01F	109.6(10)
N00E–C01I	1.474(13)	C010–N00C–C00Q	112.5(7)
N00E–C01J	1.450(14)	C010–N00C–C015	108.9(8)
N00E–C01L	1.502(13)	C010–N00C–C017	110.0(8)
N00F–C00M	1.525(11)	C015–N00C–C00Q	109.4(8)
N00F–C014	1.545(14)	C017–N00C–C00Q	105.5(7)

N00F-C01D	1.493(13)	C017-N00C-C015	110.5(8)
N00F-C01E	1.503(14)	C01I-N00E-C00R	108.3(7)
F00G-C00Y	1.325(12)	C01I-N00E-C01L	106.2(10)
F00H-C019	1.339(17)	C01J-N00E-C00R	110.5(8)
F00I-C011	1.357(13)	C01J-N00E-C01I	108.8(10)
C00J-C00P	1.411(13)	C01J-N00E-C01L	112.6(11)
C00J-C00S	1.496(13)	C01L-N00E-C00R	110.2(8)
C00J-C00Y	1.362(14)	C00M-N00F-C014	105.0(8)
C00K-C00R	1.485(12)	C01D-N00F-C00M	111.5(8)
C00K-C00X	1.380(15)	C01D-N00F-C014	110.0(9)
C00K-C018	1.279(14)	C01D-N00F-C01E	109.7(9)
F00L-C018	1.361(15)	C01E-N00F-C00M	111.2(8)
C00M-C00O	1.496(12)	C01E-N00F-C014	109.3(9)
F00N-C01G	1.324(18)	C00P-C00J-C00S	119.1(9)
C00O-C011	1.322(14)	C00Y-C00J-C00P	118.1(9)
C00O-C01B	1.375(14)	C00Y-C00J-C00S	122.6(9)
C00P-C00V	1.376(14)	C00X-C00K-C00R	119.5(9)
C00Q-C00U	1.501(13)	C018-C00K-C00R	122.2(10)
F00T-C00Z	1.384(15)	C018-C00K-C00X	117.9(10)
C00U-C00W	1.451(17)	C00O-C00M-N00F	114.3(7)
C00U-C019	1.352(17)	C011-C00O-C00M	122.9(9)
C00V-C013	1.383(18)	C011-C00O-C01B	117.6(10)
C00W-C01G	1.338(18)	C01B-C00O-C00M	119.4(9)
C00X-C00Z	1.366(15)	C00V-C00P-C00J	117.2(10)
C00Y-C01A	1.404(17)	C00U-C00Q-N00C	114.4(7)
C00Z-C01K	1.315(18)	C00K-C00R-N00E	115.9(7)
C011-C016	1.426(16)	C00J-C00S-N00B	114.9(7)
C013-C01A	1.387(19)	C00W-C00U-C00Q	115.7(11)
C016-C01C	1.37(2)	C019-C00U-C00Q	123.3(11)
C018-C01Q	1.454(18)	C019-C00U-C00W	120.6(11)
C019-C01P	1.359(19)	F00D-C00V-C00P	116.6(11)
C01B-C01O	1.347(18)	F00D-C00V-C013	118.2(11)
C01C-C01O	1.38(2)	C00P-C00V-C013	124.9(11)
C01G-C01N	1.50(3)	C01G-C00W-C00U	115.8(15)
F01H-C01O	1.329(18)	C00Z-C00X-C00K	117.7(11)
C01K-C01Q	1.41(2)	F00G-C00Y-C00J	118.8(10)
C01N-C01P	1.37(3)	F00G-C00Y-C01A	117.0(11)
		C00J-C00Y-C01A	124.2(11)
		C00X-C00Z-F00T	116.5(12)
		C01K-C00Z-F00T	116.6(12)
		C01K-C00Z-C00X	126.8(13)
		F00I-C011-C016	116.3(11)
		C00O-C011-F00I	119.2(10)
		C00O-C011-C016	124.4(12)
		C01A-C013-C00V	117.5(11)
		C01C-C016-C011	116.4(13)
		C00K-C018-F00L	119.3(11)
		C00K-C018-C01Q	125.8(13)
		F00L-C018-C01Q	114.8(11)
		F00H-C019-C00U	119.2(11)
		F00H-C019-C01P	115.8(15)
		C01P-C019-C00U	125.0(16)
		C013-C01A-C00Y	117.8(12)
		C01O-C01B-C00O	120.0(13)
		C016-C01C-C01O	118.6(13)
		F00N-C01G-C00W	120.5(19)
		F00N-C01G-C01N	117.1(14)

C00W–C01G–C01N	122.1(16)
C00Z–C01K–C01Q	117.0(12)
C01P–C01N–C01G	118.7(13)
C01B–C01O–C01C	122.8(15)
F01H–C01O–C01B	122.1(17)
F01H–C01O–C01C	115.0(14)
C019–C01P–C01N	117.4(17)
C01K–C01Q–C018	114.6(12)

Table S6 The bond lengths (Å) and angles (°) of FBTAM-Cl in the HTP.

Atom–Atom	Length [Å]	Atom–Atom–Atom	Angle [°]
Mn1–Cl1	2.431(4)	Cl1–Mn1–Cl4	110.02(18)
Mn1–Cl4	2.436(5)	Cl2–Mn1–Cl1	113.54(17)
Mn1–Cl2	2.405(4)	Cl2–Mn1–Cl4	107.73(19)
Mn1–Cl3	2.417(5)	Cl2–Mn1–Cl3	107.3(2)
N1–C4	1.523(18)	Cl3–Mn1–Cl1	109.4(2)
N1–C22	1.49(2)	Cl3–Mn1–Cl4	108.7(2)
N1–C24	1.50(2)	C22–N1–C4	97(3)
N1–C26	1.49(2)	C22–N1–C13	113(3)
N1–C13	1.51(2)	C24–N1–C4	116.4(19)
N1–C7	1.49(2)	C26–N1–C4	108.0(19)
N1–C15	1.49(2)	C26–N1–C24	108(2)
N2–C14	1.539(19)	C26–N1–C7	102(3)
N2–C16	1.558(17)	C13–N1–C4	105(3)
N2–C18	1.50(2)	C7–N1–C4	114(2)
N2–C11	1.533(18)	C7–N1–C24	107(3)
N2–C23	1.55(2)	C15–N1–C4	109(3)
N2–C3	1.58(2)	C15–N1–C22	118(4)
N2–C25	1.59(2)	C15–N1–C13	112(3)
C1–C4	1.51(3)	C14–N2–C23	91.5(19)
C1–C8	1.36(3)	C14–N2–C3	134(4)
C1–C20	1.49(3)	C16–N2–C25	93.7(16)
F1–C20	1.45(3)	C18–N2–C14	106(3)
C4–H4A	0.9700	C18–N2–C16	140(3)
C4–H4B	0.9700	C18–N2–C11	100(2)
C6–H6	0.9300	C18–N2–C23	136(4)
C6–C10	1.32(3)	C18–N2–C3	102(3)
C6–C12	1.28(3)	C18–N2–C25	106(3)
F4–C12	1.47(3)	C11–N2–C16	97.8(18)
C8–H8	0.9300	C11–N2–C25	122(4)
C8–C12	1.34(3)	C23–N2–C3	93(3)
C10–H10	0.9300	C8–C1–C4	124(2)
C10–C20	1.29(3)	C8–C1–C20	113(2)
C12–F6	1.50(4)	C20–C1–C4	123(2)
C14–H14A	0.9600	N1–C4–H4A	107.9
C14–H14B	0.9601	N1–C4–H4B	107.9
C14–H14C	0.9600	C1–C4–N1	117.7(18)
C16–H16A	0.9603	C1–C4–H4A	107.9
C16–H16B	0.9601	C1–C4–H4B	107.9
C16–H16C	0.9600	H4A–C4–H4B	107.2
C18–H18A	0.9700	C10–C6–H6	119.3
C18–H18B	0.9700	C12–C6–H6	119.3
C18–C5	1.60(2)	C12–C6–C10	121(2)
C20–F8	1.44(4)	C1–C8–H8	120.8
C22–H22A	0.9600	C12–C8–C1	118(2)
C22–H22B	0.9600	C12–C8–H8	120.8

C22-H22C	0.9600	C6-C10-H10	121.2
C24-H24A	0.9600	C20-C10-C6	118(3)
C24-H24B	0.9598	C20-C10-H10	121.2
C24-H24C	0.9603	C6-C12-F4	122(3)
C26-H26A	0.9596	C6-C12-C8	125(3)
C26-H26B	0.9595	C6-C12-F6	110(3)
C26-H26C	0.9601	C8-C12-F4	111(3)
C13-H13A	0.9603	C8-C12-F6	119(3)
C13-H13B	0.9599	N2-C14-H14A	98.7
C13-H13C	0.9603	N2-C14-H14B	107.2
C7-H7A	0.9599	N2-C14-H14C	121.8
C7-H7B	0.9601	H14A-C14-H14B	109.5
C7-H7C	0.9596	H14A-C14-H14C	109.5
C15-H15A	0.9601	H14B-C14-H14C	109.4
C15-H15B	0.9596	N2-C16-H16A	112.0
C15-H15C	0.9595	N2-C16-H16B	121.4
C2-H2	0.9300	N2-C16-H16C	93.5
C2-C17	1.3900	H16A-C16-H16B	109.5
C2-C21	1.3900	H16A-C16-H16C	109.5
C17-H17	0.9300	H16B-C16-H16C	109.5
C17-C9	1.3900	N2-C18-H18A	109.2
C9-C19	1.3900	N2-C18-H18B	109.2
C9-F5	1.428(18)	N2-C18-C5	112(2)
C9-F3	1.43(2)	H18A-C18-H18B	107.9
C19-H19	0.9300	C5-C18-H18A	109.2
C19-C5	1.3900	C5-C18-H18B	109.2
C5-C21	1.3900	F1-C20-C1	105(2)
C21-F2	1.437(19)	C10-C20-C1	124(3)
C21-F7	1.44(3)	C10-C20-F1	131(3)
C11-H11A	0.9599	C10-C20-F8	103(3)
C11-H11B	0.9596	F8-C20-C1	132(3)
C11-H11C	0.9607	N1-C22-H22A	109.5
C23-H23A	0.9601	N1-C22-H22B	109.5
C23-H23B	0.9599	N1-C22-H22C	109.5
C23-H23C	0.9604	H22A-C22-H22B	109.5
C3-H3A	0.9600	H22A-C22-H22C	109.5
C3-H3B	0.9599	H22B-C22-H22C	109.5
C3-H3C	0.9599	N1-C24-H24A	107.6
C25-H25A	0.9601	N1-C24-H24B	111.9
C25-H25B	0.9600	N1-C24-H24C	108.8
C25-H25C	0.9599	H24A-C24-H24B	109.5
		H24A-C24-H24C	109.5
		H24B-C24-H24C	109.5
		N1-C26-H26A	111.0
		N1-C26-H26B	110.4
		N1-C26-H26C	107.0
		H26A-C26-H26B	109.5
		H26A-C26-H26C	109.5
		H26B-C26-H26C	109.5
		N1-C13-H13A	105.2
		N1-C13-H13B	110.1
		N1-C13-H13C	113.0
		H13A-C13-H13B	109.5
		H13A-C13-H13C	109.4
		H13B-C13-H13C	109.5
		N1-C7-H7A	112.4
		N1-C7-H7B	107.4

N1-C7-H7C	108.5
H7A-C7-H7B	109.5
H7A-C7-H7C	109.5
H7B-C7-H7C	109.5
N1-C15-H15A	111.4
N1-C15-H15B	114.3
N1-C15-H15C	102.3
H15A-C15-H15B	109.5
H15A-C15-H15C	109.5
H15B-C15-H15C	109.6
C17-C2-H2	120.0
C17-C2-C21	120.0
C21-C2-H2	120.0
C2-C17-H17	120.0
C9-C17-C2	120.0
C9-C17-H17	120.0
C17-C9-C19	120.0
C17-C9-F5	110(2)
C17-C9-F3	119(3)
C19-C9-F5	127(2)
C19-C9-F3	103(3)
C9-C19-H19	120.0
C5-C19-C9	120.0
C5-C19-H19	120.0
C19-C5-C18	107.9(17)
C19-C5-C21	120.0
C21-C5-C18	132.1(17)
C2-C21-F2	98(2)
C2-C21-F7	132(3)
C5-C21-C2	120.0
C5-C21-F2	122(3)
C5-C21-F7	101(3)
N2-C11-H11A	91.8
N2-C11-H11B	135.9
N2-C11-H11C	98.1
H11A-C11-H11B	109.5
H11A-C11-H11C	109.4
H11B-C11-H11C	109.5
N2-C23-H23A	112.1
N2-C23-H23B	120.8
N2-C23-H23C	94.1
H23A-C23-H23B	109.5
H23A-C23-H23C	109.5
H23B-C23-H23C	109.4
N2-C3-H3A	106.8
N2-C3-H3B	117.9
N2-C3-H3C	103.4
H3A-C3-H3B	109.5
H3A-C3-H3C	109.5
H3B-C3-H3C	109.5
N2-C25-H25A	84.9
N2-C25-H25B	122.6
N2-C25-H25C	117.3
H25A-C25-H25B	109.5
H25A-C25-H25C	109.5
H25B-C25-H25C	109.5

Table S7 The distance between adjacent inorganic frameworks of FBTAM-Cl in the LTP and HTP.

	FBTAM-Cl (302K)	FBTAM-Cl (433K)
Inorganic skeleton distance	11.0045(24)	8.6781(19)
Inorganic skeleton distance	11.3813(37)	8.8604(40)

Table S8 Crystal data and structure refinements for FBTAM-I in the LTP.

FBTAM-I (301K)	
Empirical formula	C ₈₀ H ₁₁₂ F ₁₆ I ₁₆ Mn ₄ N ₈
Formula weight	3739.93
Space group	$P\bar{1}$ (2)
Crystal system	triclinic
a/ Å	10.5000(4)
b/ Å	18.0029(7)
c/ Å	31.9824(8)
α/°	101.214(3)
β/°	92.164(2)
γ/°	93.299(3)
Volume/ Å³	5913.0(4)
Z	2
F(000)	3480
GOF	0.813
R_{int}	0.0685
R₁	0.0491
wR₂	0.1265

Table S9 The bond lengths (Å) and angles (°) of FBTAM-I in the LTP.

Atom–Atom	Length [Å]	Atom–Atom–Atom	Angle [°]
I10–Mn3	2.7195(13)	I10–Mn3–I9	107.59(4)
I4–Mn1	2.6727(14)	I12–Mn3–I10	109.81(5)
I14–Mn4	2.6589(14)	I12–Mn3–I9	109.68(5)
I13–Mn4	2.7184(14)	I12–Mn3–I11	107.63(5)
I2–Mn1	2.7460(13)	I11–Mn3–I10	111.40(5)
I9–Mn3	2.7284(13)	I11–Mn3–I9	110.73(5)
I12–Mn3	2.6794(14)	I14–Mn4–I13	108.74(5)
I5–Mn2	2.7036(14)	I14–Mn4–I15	111.64(5)
I15–Mn4	2.6776(13)	I14–Mn4–I16	109.17(5)
I8–Mn2	2.7384(14)	I15–Mn4–I13	108.92(5)
I1–Mn1	2.7082(14)	I16–Mn4–I13	108.79(5)
I6–Mn2	2.6975(15)	I16–Mn4–I15	109.53(5)
I16–Mn4	2.6621(14)	I5–Mn2–I8	107.95(5)
I11–Mn3	2.6797(15)	I6–Mn2–I5	109.00(5)
I7–Mn2	2.6786(14)	I6–Mn2–I8	107.57(5)
I3–Mn1	2.6750(15)	I7–Mn2–I5	110.69(5)
F11–C26	1.372(10)	I7–Mn2–I8	110.88(5)
F6–C55	1.360(10)	I7–Mn2–I6	110.66(5)
F16–C3	1.359(10)	I4–Mn1–I2	108.35(5)
F12–C29	1.330(10)	I4–Mn1–I1	109.09(5)
F10–C35	1.348(10)	I4–Mn1–I3	108.62(5)
F3–C64	1.370(10)	I1–Mn1–I2	106.78(5)
F4–C67	1.375(10)	I3–Mn1–I2	110.03(5)
N00S–C70	1.485(10)	I3–Mn1–I1	113.84(5)
N00S–C71	1.505(11)	C70–N00S–C71	108.5(7)
N00S–C68	1.541(10)	C70–N00S–C68	111.5(6)

N00S-C69	1.490(11)	C70-N00S-C69	109.6(7)
N00T-C24	1.528(9)	C71-N00S-C68	107.0(7)
N00T-C21	1.484(11)	C69-N00S-C71	108.4(7)
N00T-C23	1.492(11)	C69-N00S-C68	111.7(7)
N00T-C22	1.494(11)	C21-N00T-C24	112.0(7)
F2-C52	1.342(10)	C21-N00T-C23	109.4(7)
N00V-C20	1.501(11)	C21-N00T-C22	108.5(7)
N00V-C17	1.529(10)	C23-N00T-C24	110.1(6)
N00V-C19	1.506(11)	C23-N00T-C22	111.0(8)
N00V-C18	1.488(11)	C22-N00T-C24	105.8(7)
F8-C51	1.352(11)	C20-N00V-C17	110.6(7)
F5-C81	1.342(11)	C20-N00V-C19	108.5(7)
F9-C32	1.370(11)	C19-N00V-C17	106.9(7)
F1-C78	1.329(11)	C18-N00V-C20	109.4(7)
F14-C15	1.362(11)	C18-N00V-C17	111.9(7)
F13-C12	1.373(11)	C18-N00V-C19	109.4(7)
F15-C6	1.376(11)	C74-N014-C75	110.7(7)
F7-C48	1.369(11)	C74-N014-C73	107.2(8)
N014-C75	1.538(11)	C72-N014-C75	110.6(7)
N014-C74	1.482(11)	C72-N014-C74	110.2(8)
N014-C72	1.469(11)	C72-N014-C73	110.8(8)
N014-C73	1.509(12)	C73-N014-C75	107.2(8)
N015-C38	1.523(11)	C41-N015-C38	111.8(7)
N015-C41	1.502(12)	C40-N015-C38	110.8(8)
N015-C40	1.483(12)	C40-N015-C41	109.5(8)
N015-C39	1.494(12)	C40-N015-C39	108.6(8)
N016-C58	1.524(11)	C39-N015-C38	107.2(7)
N016-C61	1.506(10)	C39-N015-C41	108.9(9)
N016-C59	1.478(12)	C61-N016-C58	110.5(7)
N016-C60	1.512(12)	C61-N016-C60	108.2(7)
N017-C7	1.521(11)	C59-N016-C58	110.2(7)
N017-C8	1.477(12)	C59-N016-C61	110.1(8)
N017-C10	1.467(12)	C59-N016-C60	110.7(8)
N017-C9	1.460(13)	C60-N016-C58	107.1(8)
C25-C26	1.369(11)	C8-N017-C7	110.6(7)
C25-C30	1.382(11)	C10-N017-C7	112.3(7)
C25-C24	1.508(11)	C10-N017-C8	108.2(9)
N019-C45	1.514(11)	C9-N017-C7	107.4(8)
N019-C43	1.492(12)	C9-N017-C8	108.1(9)
N019-C42	1.478(12)	C9-N017-C10	110.2(9)
N019-C44	1.484(12)	C26-C25-C30	116.4(8)
C65-C66	1.389(11)	C26-C25-C24	122.5(8)
C65-C68	1.484(11)	C30-C25-C24	121.1(7)
C65-C64	1.361(12)	C43-N019-C45	107.5(7)
C66-H66	0.9300	C42-N019-C45	110.7(8)
C66-C67	1.371(13)	C42-N019-C43	108.3(8)
C14-C13	1.397(12)	C42-N019-C44	108.8(9)
C14-C17	1.484(11)	C44-N019-C45	112.2(8)
C14-C15	1.376(12)	C44-N019-C43	109.3(9)
C36-C38	1.493(11)	C66-C65-C68	122.5(8)
C36-C37	1.386(12)	C64-C65-C66	115.5(8)
C36-C35	1.393(11)	C64-C65-C68	121.9(8)
C26-C27	1.345(13)	C65-C66-H66	120.5
C30-H30	0.9300	C67-C66-C65	119.1(8)
C30-C29	1.362(12)	C67-C66-H66	120.5
C56-C58	1.492(12)	C13-C14-C17	121.8(8)
C56-C55	1.385(12)	C15-C14-C13	115.6(8)

C56-C57	1.395(12)	C15-C14-C17	122.4(8)
C24-H24A	0.9700	C37-C36-C38	120.9(7)
C24-H24B	0.9700	C37-C36-C35	115.4(8)
C4-C3	1.362(13)	C35-C36-C38	123.5(8)
C4-C5	1.407(12)	C25-C26-F11	117.8(8)
C4-C7	1.482(13)	C27-C26-F11	118.4(8)
C46-C45	1.503(12)	C27-C26-C25	123.8(9)
C46-C47	1.371(12)	C25-C30-H30	119.8
C46-C51	1.383(13)	C29-C30-C25	120.4(8)
C13-H13	0.9300	C29-C30-H30	119.8
C13-C12	1.351(13)	C55-C56-C58	123.3(8)
C38-H38A	0.9700	C55-C56-C57	115.9(8)
C38-H38B	0.9700	C57-C56-C58	120.8(8)
C3-C2	1.374(13)	N00T-C24-H24A	108.7
C70-H70A	0.9600	N00T-C24-H24B	108.7
C70-H70B	0.9600	C25-C24-N00T	114.3(7)
C70-H70C	0.9600	C25-C24-H24A	108.7
C37-H37	0.9300	C25-C24-H24B	108.7
C37-C32	1.368(12)	H24A-C24-H24B	107.6
C71-H71A	0.9600	C3-C4-C5	115.5(9)
C71-H71B	0.9600	C3-C4-C7	123.9(8)
C71-H71C	0.9600	C5-C4-C7	120.5(9)
C35-C34	1.355(13)	C47-C46-C45	120.5(9)
C77-H77	0.9300	C47-C46-C51	116.2(8)
C77-C76	1.380(12)	C51-C46-C45	123.3(9)
C77-C78	1.345(13)	C14-C13-H13	120.7
C32-C33	1.344(14)	C12-C13-C14	118.6(8)
C21-H21A	0.9600	C12-C13-H13	120.7
C21-H21B	0.9600	N015-C38-H38A	108.8
C21-H21C	0.9600	N015-C38-H38B	108.8
C5-H5	0.9300	C36-C38-N015	113.8(6)
C5-C6	1.380(14)	C36-C38-H38A	108.8
C58-H58A	0.9700	C36-C38-H38B	108.8
C58-H58B	0.9700	H38A-C38-H38B	107.7
C55-C54	1.362(13)	F16-C3-C4	118.3(8)
C27-H27	0.9300	F16-C3-C2	116.2(9)
C27-C28	1.367(14)	C4-C3-C2	125.5(9)
C68-H68A	0.9700	N00S-C70-H70A	109.5
C68-H68B	0.9700	N00S-C70-H70B	109.5
C57-H57	0.9300	N00S-C70-H70C	109.5
C57-C52	1.385(13)	H70A-C70-H70B	109.5
C75-H75A	0.9700	H70A-C70-H70C	109.5
C75-H75B	0.9700	H70B-C70-H70C	109.5
C75-C76	1.488(13)	C36-C37-H37	119.8
C20-H20A	0.9600	C32-C37-C36	120.4(9)
C20-H20B	0.9600	C32-C37-H37	119.8
C20-H20C	0.9600	N00S-C71-H71A	109.5
C76-C81	1.385(13)	N00S-C71-H71B	109.5
C17-H17A	0.9700	N00S-C71-H71C	109.5
C17-H17B	0.9700	H71A-C71-H71B	109.5
C67-C62	1.341(14)	H71A-C71-H71C	109.5
C54-H54	0.9300	H71B-C71-H71C	109.5
C54-C53	1.365(14)	F10-C35-C36	116.9(8)
C29-C28	1.384(13)	F10-C35-C34	119.9(8)
C34-H34	0.9300	C34-C35-C36	123.0(9)
C34-C33	1.357(15)	C76-C77-H77	119.2
C45-H45A	0.9700	C78-C77-H77	119.2

C45-H45B	0.9700	C78-C77-C76	121.6(9)
C28-H28	0.9300	C37-C32-F9	118.0(9)
C12-C11	1.338(14)	C33-C32-F9	119.3(9)
C64-C63	1.360(13)	C33-C32-C37	122.6(10)
C49-H49	0.9300	N00T-C21-H21A	109.5
C49-C50	1.374(15)	N00T-C21-H21B	109.5
C49-C48	1.336(14)	N00T-C21-H21C	109.5
C47-H47	0.9300	H21A-C21-H21B	109.5
C47-C48	1.372(13)	H21A-C21-H21C	109.5
C61-H61A	0.9600	H21B-C21-H21C	109.5
C61-H61B	0.9600	C4-C5-H5	120.8
C61-H61C	0.9600	C6-C5-C4	118.4(10)
C51-C50	1.359(14)	C6-C5-H5	120.8
C7-H7A	0.9700	N016-C58-H58A	108.4
C7-H7B	0.9700	N016-C58-H58B	108.4
C52-C53	1.387(14)	C56-C58-N016	115.3(7)
C15-C16	1.373(14)	C56-C58-H58A	108.4
C19-H19A	0.9600	C56-C58-H58B	108.4
C19-H19B	0.9600	H58A-C58-H58B	107.5
C19-H19C	0.9600	F6-C55-C56	117.5(8)
C2-H2	0.9300	F6-C55-C54	117.9(9)
C2-C1	1.365(15)	C54-C55-C56	124.6(8)
C33-H33	0.9300	C26-C27-H27	120.0
C50-H50	0.9300	C26-C27-C28	119.9(9)
C74-H74A	0.9600	C28-C27-H27	120.0
C74-H74B	0.9600	N00S-C68-H68A	108.7
C74-H74C	0.9600	N00S-C68-H68B	108.7
C23-H23A	0.9600	C65-C68-N00S	114.3(7)
C23-H23B	0.9600	C65-C68-H68A	108.7
C23-H23C	0.9600	C65-C68-H68B	108.7
C62-H62	0.9300	H68A-C68-H68B	107.6
C62-C63	1.347(14)	C56-C57-H57	120.1
C79-H79	0.9300	C52-C57-C56	119.8(8)
C79-C78	1.360(14)	C52-C57-H57	120.1
C79-C80	1.363(15)	N014-C75-H75A	108.5
C53-H53	0.9300	N014-C75-H75B	108.5
C6-C1	1.351(16)	H75A-C75-H75B	107.5
C16-H16	0.9300	C76-C75-N014	115.1(7)
C16-C11	1.360(15)	C76-C75-H75A	108.5
C1-H1	0.9300	C76-C75-H75B	108.5
C41-H41A	0.9600	N00V-C20-H20A	109.5
C41-H41B	0.9600	N00V-C20-H20B	109.5
C41-H41C	0.9600	N00V-C20-H20C	109.5
C59-H59A	0.9600	H20A-C20-H20B	109.5
C59-H59B	0.9600	H20A-C20-H20C	109.5
C59-H59C	0.9600	H20B-C20-H20C	109.5
C81-C80	1.370(15)	C77-C76-C75	122.2(9)
C69-H69A	0.9600	C77-C76-C81	116.3(10)
C69-H69B	0.9600	C81-C76-C75	121.5(9)
C69-H69C	0.9600	N00V-C17-H17A	108.8
C18-H18A	0.9600	N00V-C17-H17B	108.8
C18-H18B	0.9600	C14-C17-N00V	114.0(7)
C18-H18C	0.9600	C14-C17-H17A	108.8
C22-H22A	0.9600	C14-C17-H17B	108.8
C22-H22B	0.9600	H17A-C17-H17B	107.7
C22-H22C	0.9600	C66-C67-F4	116.2(9)
C63-H63	0.9300	C62-C67-F4	120.9(10)

C8-H8A	0.9600	C62-C67-C66	122.8(9)
C8-H8B	0.9600	C55-C54-H54	120.4
C8-H8C	0.9600	C55-C54-C53	119.1(9)
C11-H11	0.9300	C53-C54-H54	120.4
C80-H80	0.9300	F12-C29-C30	119.2(9)
C10-H10A	0.9600	F12-C29-C28	118.9(9)
C10-H10B	0.9600	C30-C29-C28	121.8(9)
C10-H10C	0.9600	C35-C34-H34	120.0
C40-H40A	0.9600	C35-C34-C33	120.0(9)
C40-H40B	0.9600	C33-C34-H34	120.0
C40-H40C	0.9600	N019-C45-H45A	108.3
C43-H43A	0.9600	N019-C45-H45B	108.3
C43-H43B	0.9600	C46-C45-N019	115.8(7)
C43-H43C	0.9600	C46-C45-H45A	108.3
C60-H60A	0.9600	C46-C45-H45B	108.3
C60-H60B	0.9600	H45A-C45-H45B	107.4
C60-H60C	0.9600	C27-C28-C29	117.6(9)
C72-H72A	0.9600	C27-C28-H28	121.2
C72-H72B	0.9600	C29-C28-H28	121.2
C72-H72C	0.9600	C13-C12-F13	116.5(9)
C39-H39A	0.9600	C11-C12-F13	118.2(10)
C39-H39B	0.9600	C11-C12-C13	125.2(9)
C39-H39C	0.9600	C65-C64-F3	118.3(8)
C42-H42A	0.9600	C63-C64-F3	116.3(8)
C42-H42B	0.9600	C63-C64-C65	125.3(8)
C42-H42C	0.9600	C50-C49-H49	121.0
C73-H73A	0.9600	C48-C49-H49	121.0
C73-H73B	0.9600	C48-C49-C50	117.9(10)
C73-H73C	0.9600	C46-C47-H47	120.3
C44-H44A	0.9600	C46-C47-C48	119.5(10)
C44-H44B	0.9600	C48-C47-H47	120.3
C44-H44C	0.9600	N016-C61-H61A	109.5
C9-H9A	0.9600	N016-C61-H61B	109.5
C9-H9B	0.9600	N016-C61-H61C	109.5
C9-H9C	0.9600	H61A-C61-H61B	109.5
		H61A-C61-H61C	109.5
		H61B-C61-H61C	109.5
		F8-C51-C46	117.9(9)
		F8-C51-C50	118.3(10)
		C50-C51-C46	123.6(10)
		N017-C7-H7A	108.8
		N017-C7-H7B	108.8
		C4-C7-N017	113.8(8)
		C4-C7-H7A	108.8
		C4-C7-H7B	108.8
		H7A-C7-H7B	107.7
		F2-C52-C57	117.8(9)
		F2-C52-C53	120.2(9)
		C57-C52-C53	122.0(9)
		F14-C15-C14	117.9(8)
		F14-C15-C16	118.1(9)
		C16-C15-C14	124.0(9)
		N00V-C19-H19A	109.5
		N00V-C19-H19B	109.5
		N00V-C19-H19C	109.5
		H19A-C19-H19B	109.5
		H19A-C19-H19C	109.5

H19B-C19-H19C	109.5
C3-C2-H2	120.9
C1-C2-C3	118.1(10)
C1-C2-H2	120.9
C32-C33-C34	118.5(10)
C32-C33-H33	120.8
C34-C33-H33	120.8
C49-C50-H50	120.5
C51-C50-C49	119.0(11)
C51-C50-H50	120.5
N014-C74-H74A	109.5
N014-C74-H74B	109.5
N014-C74-H74C	109.5
H74A-C74-H74B	109.5
H74A-C74-H74C	109.5
H74B-C74-H74C	109.5
N00T-C23-H23A	109.5
N00T-C23-H23B	109.5
N00T-C23-H23C	109.5
H23A-C23-H23B	109.5
H23A-C23-H23C	109.5
H23B-C23-H23C	109.5
C67-C62-H62	120.2
C67-C62-C63	119.5(10)
C63-C62-H62	120.2
C78-C79-H79	119.5
C78-C79-C80	121.0(11)
C80-C79-H79	119.5
F7-C48-C47	116.5(10)
C49-C48-F7	119.7(9)
C49-C48-C47	123.8(10)
C54-C53-C52	118.5(10)
C54-C53-H53	120.8
C52-C53-H53	120.8
F15-C6-C5	116.7(11)
C1-C6-F15	119.4(10)
C1-C6-C5	123.9(10)
C15-C16-H16	120.6
C11-C16-C15	118.7(9)
C11-C16-H16	120.6
C2-C1-H1	120.9
C6-C1-C2	118.2(10)
C6-C1-H1	120.9
N015-C41-H41A	109.5
N015-C41-H41B	109.5
N015-C41-H41C	109.5
H41A-C41-H41B	109.5
H41A-C41-H41C	109.5
H41B-C41-H41C	109.5
N016-C59-H59A	109.5
N016-C59-H59B	109.5
N016-C59-H59C	109.5
H59A-C59-H59B	109.5
H59A-C59-H59C	109.5
H59B-C59-H59C	109.5
F5-C81-C76	119.1(10)
F5-C81-C80	118.1(10)

C80-C81-C76	122.8(10)
N00S-C69-H69A	109.5
N00S-C69-H69B	109.5
N00S-C69-H69C	109.5
H69A-C69-H69B	109.5
H69A-C69-H69C	109.5
H69B-C69-H69C	109.5
N00V-C18-H18A	109.5
N00V-C18-H18B	109.5
N00V-C18-H18C	109.5
H18A-C18-H18B	109.5
H18A-C18-H18C	109.5
H18B-C18-H18C	109.5
N00T-C22-H22A	109.5
N00T-C22-H22B	109.5
N00T-C22-H22C	109.5
H22A-C22-H22B	109.5
H22A-C22-H22C	109.5
H22B-C22-H22C	109.5
C64-C63-H63	121.1
C62-C63-C64	117.7(10)
C62-C63-H63	121.1
F1-C78-C77	119.8(9)
F1-C78-C79	119.8(10)
C77-C78-C79	120.4(10)
N017-C8-H8A	109.5
N017-C8-H8B	109.5
N017-C8-H8C	109.5
H8A-C8-H8B	109.5
H8A-C8-H8C	109.5
H8B-C8-H8C	109.5
C12-C11-C16	117.7(9)
C12-C11-H11	121.2
C16-C11-H11	121.2
C79-C80-C81	117.8(11)
C79-C80-H80	121.1
C81-C80-H80	121.1
N017-C10-H10A	109.5
N017-C10-H10B	109.5
N017-C10-H10C	109.5
H10A-C10-H10B	109.5
H10A-C10-H10C	109.5
H10B-C10-H10C	109.5
N015-C40-H40A	109.5
N015-C40-H40B	109.5
N015-C40-H40C	109.5
H40A-C40-H40B	109.5
H40A-C40-H40C	109.5
H40B-C40-H40C	109.5
N019-C43-H43A	109.5
N019-C43-H43B	109.5
N019-C43-H43C	109.5
H43A-C43-H43B	109.5
H43A-C43-H43C	109.5
H43B-C43-H43C	109.5
N016-C60-H60A	109.5
N016-C60-H60B	109.5

N016-C60-H60C	109.5
H60A-C60-H60B	109.5
H60A-C60-H60C	109.5
H60B-C60-H60C	109.5
N014-C72-H72A	109.5
N014-C72-H72B	109.5
N014-C72-H72C	109.5
H72A-C72-H72B	109.5
H72A-C72-H72C	109.5
H72B-C72-H72C	109.5
N015-C39-H39A	109.5
N015-C39-H39B	109.5
N015-C39-H39C	109.5
H39A-C39-H39B	109.5
H39A-C39-H39C	109.5
H39B-C39-H39C	109.5
N019-C42-H42A	109.5
N019-C42-H42B	109.5
N019-C42-H42C	109.5
H42A-C42-H42B	109.5
H42A-C42-H42C	109.5
H42B-C42-H42C	109.5
N014-C73-H73A	109.5
N014-C73-H73B	109.5
N014-C73-H73C	109.5
H73A-C73-H73B	109.5
H73A-C73-H73C	109.5
H73B-C73-H73C	109.5
N019-C44-H44A	109.5
N019-C44-H44B	109.5
N019-C44-H44C	109.5
H44A-C44-H44B	109.5
H44A-C44-H44C	109.5
H44B-C44-H44C	109.5
N017-C9-H9A	109.5
N017-C9-H9B	109.5
N017-C9-H9C	109.5
H9A-C9-H9B	109.5
H9A-C9-H9C	109.5
H9B-C9-H9C	109.5
