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Red-light emission and dielectric reversible duple opto-electronic switches in a hybrid multifunctional material: (2-methylimidazolium)$MnCl_3(H_2O)$

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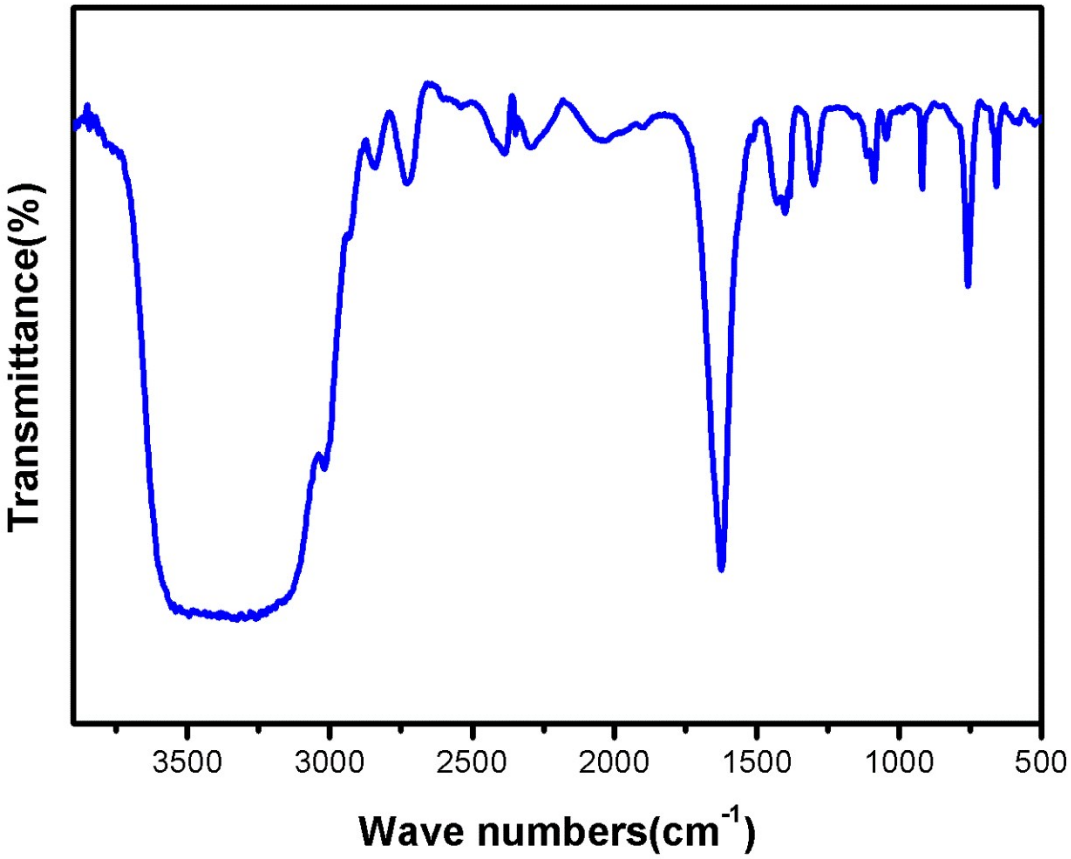

Figure S1. The IR spectrum for compound **1**

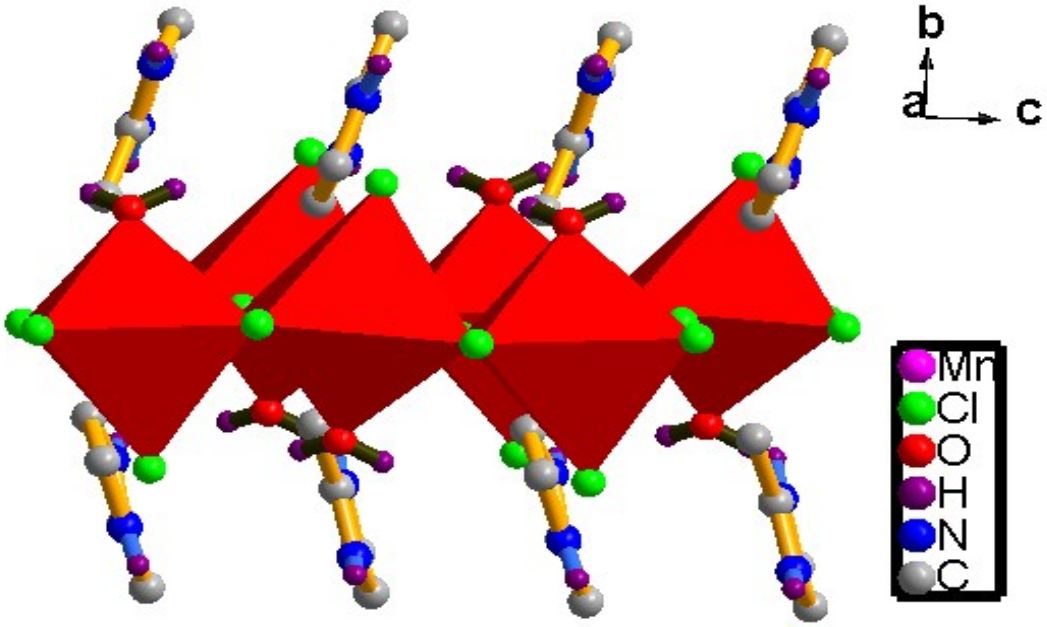

Figure S2. The packing diagram of $\{(2\text{-methylimidazolium})[MnCl_3(H_2O)]\}_n$ at 173K. All H atoms bonded to C atoms are omitted for clarity.

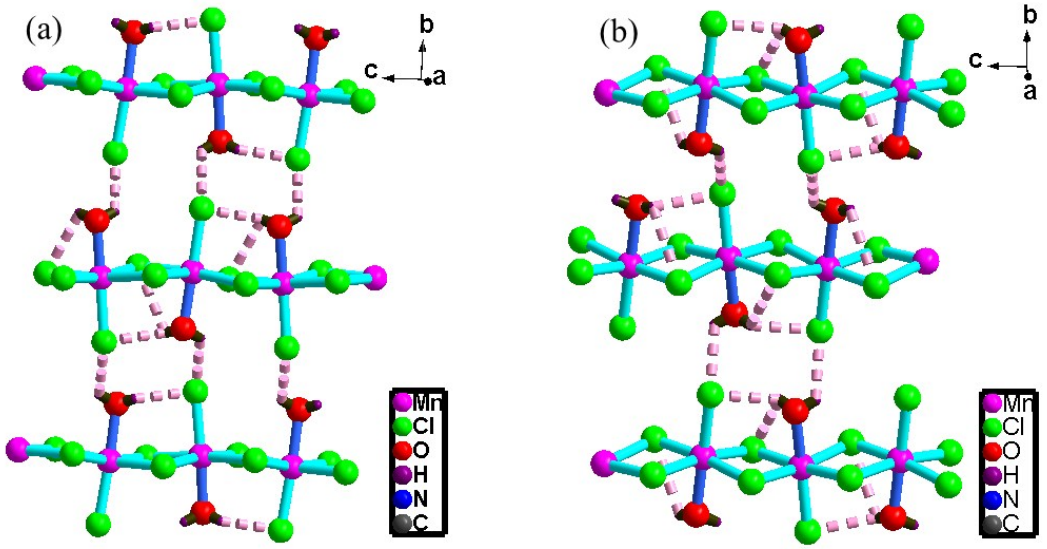

Figure S3. (a) Hydrogen bonding interactions between $[MnCl_3(H_2O)]^-$ chains at 173K.(b) Hydrogen bonding interactions between $[MnCl_3(H_2O)]^-$ chains at 293K. All H atoms bonded to C atoms are omitted for clarity.

Table S1. Crystal data and structure refinements for 1 at 293K and 173K.

	RTP(293K)	LTP(173K)
Empirical formula	$C_4H_7N_2,MnCl_3(H_2O)$	$C_4H_7N_2,MnCl_3(H_2O)$
Formula weight	262.42	262.42
Temperature(K)	293(2)	173(2)
Crystal system	Monoclinic	Monoclinic

Space group	$P2_1/c$	$P2_1/c$
a/ Å	8.9890(18)	26.896(3)
b/ Å	14.612(3)	14.523(3)
c/ Å	7.2748(15)	7.2525(10)
Volume(Å^3)	953.36(34)	2826.47(77)
Z	4	12
Radiation type	Mo-Kα	Mo-Kα
Absorption correction	Semi-empirical	Semi-empirical
F(000)	524.0	1572.0
GOF	1.062	1.178
$R_1[I > 2\sigma(I)]$	0.0798	0.0891
w$R_2[I > 2\sigma(I)]$	0.2166	0.2196

Table S2. Selected bond lengths [Å] and angles [°] for 1 at 173 and 293 K.

	293K		173K	
Bond lengths (Å)	Mn1—O1W	2.235 (9)	Mn1—O1	2.241 (6)
	Mn1—Cl2^{i}	2.500 (3)	Mn1—Cl2	2.495 (2)
	Mn1—Cl2	2.505 (3)	Mn1—Cl1	2.509 (2)
	Mn1—Cl3	2.513 (4)	Mn1—Cl2^{i}	2.509 (2)
	Mn1—Cl1^{ii}	2.559 (3)	Mn1—Cl3^{i}	2.554 (2)
	Mn1—Cl1	2.585 (3)	Mn1—Cl3	2.571 (2)
	Cl1—Mn1^{i}	2.559 (3)	Mn3—O3	2.237 (6)
	Cl2—Mn1^{ii}	2.500 (3)	Mn3—Cl7	2.504 (2)
			Mn3—Cl7^{ii}	2.508 (2)
			Mn3—Cl8	2.523 (3)
			Mn3—Cl9^{ii}	2.548 (2)
			Mn3—Cl9	2.571 (2)
			Cl9—Mn3^{iii}	2.548 (2)
			Cl3—Mn1^{iv}	2.554 (2)
			Cl7—Mn3^{iii}	2.508 (2)
			Cl2—Mn1^{iv}	2.509 (2)
			Mn2—O2	2.224 (6)
			Mn2—Cl6^{iv}	2.493 (2)
			Mn2—Cl6	2.508 (2)
			Mn2—Cl4	2.530 (2)
			Mn2—Cl5^{i}	2.554 (2)
			Mn2—Cl5	2.584 (2)
			Cl5—Mn2^{iv}	2.554 (2)
			Cl6—Mn2^{i}	2.493 (2)
Bond angles (°)	O1W—Mn1—Cl2^{i}	88.4 (3)	O1—Mn1—Cl2	87.97 (17)
	O1W—Mn1—Cl2	87.9 (3)	O1—Mn1—Cl1	175.30 (18)
	Cl2^{i}—Mn1—Cl2	93.81 (11)	Cl2—Mn1—Cl1	95.99 (8)

O1W—Mn1—Cl3	174.4 (3)	O1—Mn1—Cl2^{i}	87.15 (18)
Cl2^{i}—Mn1—Cl3	95.43 (12)	Cl2—Mn1—Cl2^{i}	93.57 (8)
Cl2—Mn1—Cl3	95.91 (12)	Cl1—Mn1—Cl2^{i}	95.11 (8)
O1W—Mn1—Cl1^{ii}	82.4 (3)	O1—Mn1—Cl3^{i}	82.69 (17)
Cl2^{i}—Mn1—Cl1^{ii}	170.61 (13)	Cl2—Mn1—Cl3^{i}	170.51 (9)
Cl2—Mn1—Cl1^{ii}	87.78 (11)	Cl1—Mn1—Cl3^{i}	93.27 (8)
Cl3—Mn1—Cl1^{ii}	93.61 (12)	Cl2^{i}—Mn1—Cl3^{i}	87.63 (8)
O1W—Mn1—Cl1	86.4 (3)	O1—Mn1—Cl3	87.17 (18)
Cl2^{i}—Mn1—Cl1	87.33 (11)	Cl2—Mn1—Cl3	87.58 (8)
Cl2—Mn1—Cl1	174.11 (13)	Cl1—Mn1—Cl3	90.46 (8)
Cl3—Mn1—Cl1	89.73 (12)	Cl2^{i}—Mn1—Cl3	174.16 (9)
Cl1^{ii}—Mn1—Cl1	90.17 (11)	Cl3^{i}—Mn1—Cl3	90.31(8)
Mn1^{i}—Cl1—Mn1	90.46 (11)	O3—Mn3—Cl7	89.27 (17)
Mn1^{ii}—Cl2—Mn1	93.72 (11)	O3—Mn3—Cl7^{ii}	89.17 (18)
		Cl7—Mn3—Cl7^{ii}	93.27 (8)
		O3—Mn3—Cl8	172.73 (17)
		Cl7—Mn3—Cl8	94.88 (8)
		Cl7^{ii}—Mn3—Cl8	96.53 (9)
		O3—Mn3—Cl9^{ii}	81.74 (17)
		Cl7—Mn3—Cl9^{ii}	170.91 (9)
		Cl7^{ii}—Mn3—Cl9^{ii}	87.98 (7)
		Cl8—Mn3—Cl9^{ii}	93.92 (8)
		O3—Mn3—Cl9	85.53 (18)
		Cl7—Mn3—Cl9	87.55 (7)
		Cl7^{ii}—Mn3—Cl9	174.63 (9)
		Cl8—Mn3—Cl9	88.69 (8)
		Cl9^{ii}—Mn3—Cl9	90.38 (7)
		Mn3^{iii}—Cl9—Mn3	90.64 (7)
		Mn1^{iv}—Cl3—Mn1	90.55 (8)
		Mn3—Cl7—Mn3^{iii}	93.12 (8)
		Mn1—Cl2—Mn1^{iv}	93.37 (8)
		O2—Mn2—Cl6^{iv}	88.69 (17)
		O2—Mn2—Cl6	87.22 (18)
		Cl6^{iv}—Mn2—Cl6	93.49 (7)
		O2—Mn2—Cl4	174.93 (16)
		Cl6^{iv}—Mn2—Cl4	95.09 (8)
		Cl6—Mn2—Cl4	95.90 (8)
		O2—Mn2—Cl5^{i}	82.48 (17)
		Cl6^{iv}—Mn2—Cl5^{i}	170.97 (9)
		Cl6—Mn2—Cl5^{i}	87.98 (7)
		Cl4—Mn2—Cl5^{i}	93.62 (7)
		O2—Mn2—Cl5	86.86 (18)
		Cl6^{iv}—Mn2—Cl5	87.64 (7)
		Cl6—Mn2—Cl5	173.95 (8)

	Cl4—Mn2—Cl5	89.92 (8)
	Cl5^{i}—Mn2—Cl5	89.99 (7)
	Mn2^{iv}—Cl5—Mn2	90.24 (7)
	Mn2^{i}—Cl6—Mn2	93.42 (7)

Symmetry codes: 173K : (i) x, −y+1/2, z−1/2; (ii) x, −y+3/2, z+1/2; (iii) x, −y+3/2, z−1/2; (iv) x, −y+1/2, z+1/2; 293K: (i) x, −y−3/2, z+1/2; (ii) x, −y−3/2, z−1/2.

Table S3. Hydrogen-Bond lengths and angles at 173 and 293 K in Compound 1.

173K	D–H···A	H···A (Å)	D···A (Å)	D–H···A (°)
	O2—H2C···Cl4^{i}	2.60	3.174 (7)	126
	O2—H2D···Cl4^{v}	2.59	3.143 (6)	124
	O1—H1C···Cl1^{i}	2.67	3.180 (6)	128
	O3—H3B···Cl8^{ii}	2.64	3.160 (7)	129
	O3—H3C···Cl1^{vi}	2.73	3.185 (6)	122
	N3—H3A···O3^{vii}	2.25	2.831 (10)	137
	N3—H3A···Cl9^{vii}	2.80	3.417 (8)	143
	N5—H5B···Cl1^{viii}	2.29	3.141 (8)	162
	N6—H6B···O1^{ix}	2.44	2.860 (10)	117
	N6—H6B···Cl3^{ix}	2.75	3.391 (8)	147
	O1—H1D···Cl8	2.70	3.152 (6)	122
	N2—H2B···Cl8	2.30	3.125 (9)	157
	N2—H2B···Cl9	2.98	3.496 (8)	119
	N4—H4D···Cl4	2.36	3.168 (8)	154
	N4—H4D···Cl5	2.99	3.518 (9)	120
	N1—H1B···O2	2.25	2.959 (11)	138
	N1—H1B···Cl5	2.66	3.362 (9)	137
293K	O1W—H1WA···Cl3^{ii}	2.63	3.202 (10)	126
	O1W—H1WB···Cl3^{iii}	2.64	3.177 (9)	122
	N2—H2A···Cl3^{iv}	2.28	3.13 (4)	170

N2'—H2'A···Cl3^{iv}	2.44	3.21 (4)	149
N2'—H2'A···Cl1^{iv}	2.91	3.47 (4)	125
N1—H1A···O1W	2.37	2.95 (5)	126
N1—H1A···Cl1	2.55	3.31 (5)	147
N1'—H1'A···O1W	2.33	2.86 (5)	132
N1'—H1'A···Cl1	2.95	3.51 (4)	138

Symmetry transformations used to generate equivalent atoms: 173K:(i) x, −y+1/2, z−1/2; (v) −x+1, y+1/2, −z+1/2; (ii) x, −y+3/2, z+1/2; (vi) x, y+1, z; (vii) x, y−1, z; (viii) x+1, y, z; (ix) −x+1, y−1/2, −z+1/2;293K: (ii) x, −y−3/2, z−1/2; (iii) −x, y−1/2, −z+1/2; (iv) −x−1, y−1/2, −z+1/2.