A Supramolecular Spin Crossover Fe(III) Complex and its Cr(III) Isomer: Stabilization of Water-Chloride Cluster within Supramolecular Host

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Table S1: Hydrogen bonding dimension of **complex 1**

D-H…A	D-H	H…A	D…A	<D-H…A	Symmetry
O1-H1…O6	0.8400	1.7500	2.583(3)	169.00	1-x,1-y,1-z
O5-H1W…Cl1	0.88(3)	2.29(3)	3.152(3)	166(3)	.
O5-H2W…Cl1	1.00(4)	2.16(4)	3.144(3)	167(4)	x,3/2-y,-1/2+z
O3-H3…Cl1	0.8400	2.2100	2.981(2)	153.00	1-x,-1/2+y,3/2-z
O7-H3W…O5	1.00(4)	1.88(4)	2.852(3)	165(4)	x,3/2-y,1/2+z
O7-H4W…O5	1.06(5)	1.77(5)	2.821(3)	176(4)	.
O6-H5W…O7	1.06(3)	1.67(3)	2.723(3)	169(3)	1-x,1-y,2-z
O6-H6W…Cl1	0.78(3)	2.55(3)	3.287(3)	159(3)	1-x,-1/2+y,3/2-z
C2-H2A…O1	0.9800	2.2400	2.696(3)	107.00	.
C4-H4C…O2	0.9800	2.5100	3.418(3)	155.00	x,y,-1+z
C6-H6A…N3	0.9900	2.2900	2.720(3)	105.00	.
C9-H9B…S2	0.9900	2.5000	3.029(3)	113.00	.
C11-H11A…O3	0.9800	2.2600	2.697(3)	106.00	.
C13-H13C…O4	0.9800	2.5500	3.497(3)	162.00	x,y,1+z
C15-H15A…N7	0.9900	2.3000	2.725(3)	105.00	.
C18-H18B…S1	0.9900	2.5100	3.037(3)	113.00	.

Table S2: Hydrogen bonding dimension of **complex 2**

D-H…A	D-H	H…A	D…A	<D-H…A	Symmetry
O1W-H1W1…Cl1	0.88(3)	2.38(3)	3.256(2)	171(3)	1-x, 1-y, 1-z
O1-H2…Cl1	0.8400	2.2100	2.959(2)	148.00	x, y, 1+z
O1W-H2W1…O2W	0.900(16)	1.910(17)	2.717(3)	148(2)	x, 1/2-y, 1/2+z
O2W-H1W2…O3W	0.954(16)	1.905(17)	2.855(3)	173.4(14)	1-x, 1-y, 1-z
O3-H4…O1W	0.8400	1.7500	2.559(3)	161.00	.
O2W-H2W2…O3W	0.99(2)	1.81(2)	2.798(3)	176.3(14)	1-x,-1/2+y,1/2-z
O3W-H1W3…Cl1	1.02(3)	2.17(2)	3.176(3)	170.3(11)	x, 3/2-y, 1/2+z
O3W-H2W3…Cl1	1.054(19)	2.065(17)	3.107(3)	169.4(18)	x, y, 1+z
C2-H2C…O1	0.9800	2.2600	2.695(3)	106.00	.
C4-H4A…O2	0.9800	2.5000	3.468(3)	169.00	x, y, 1+z
C6-H6A…S2	0.9900	2.5200	3.038(3)	113.00	.
C9-H9B…N3	0.9900	2.3200	2.729(3)	104.00	.
C11-H11A…O3	0.9800	2.2800	2.713(3)	106.00	.
C13-H13A…O4	0.9800	2.4700	3.409(3)	161.00	x, y ,-1+z

C15-H15A…S1	0.9900	2.5100	3.028(3)	112.00	.
C18-H18B…N7	0.9900	2.3200	2.725(3)	104.00	.

Table S3: MP2 OPTIMISED COORDINATES of Water Chloride CLUSTER FOR **Complex1**

Atom	X	Y	Z
Cl	0.	0.	0.
Cl	0.	0.	5.59062374
Cl	5.5899573606	0.	-0.0862645
O	2.808435138	-1.319444729	0.5527142641
O	-0.5959826164	-1.3194443944	2.7910509387
O	0.1988251922	-2.4363780165	-2.1966530099
O	2.1933239162	-2.4363777101	5.3579274572
O	1.805089082	-2.8552658784	2.6954810616
O	2.8669444864	-2.8552665728	-1.8495460206
O	4.993974743	-1.3194443946	-2.8858373096
H	2.0462930934	-0.7574082619	0.4333971663
H	3.5949083295	-0.7849557442	0.5209645651
H	-0.4480717034	-0.78931036	3.5672660842
H	-0.4824754887	-0.7748116762	2.0207672764
H	1.1318596569	-2.5979773352	-2.1777662789
H	0.03278148	-1.7536385673	-1.5558592301
H	2.1760287124	-2.599138629	4.4206849923
H	1.5991938684	-1.7094728002	5.5040261036
H	2.2860681684	-2.3913208145	2.0194771841
H	0.9398779905	-2.4513470357	2.7084764348
H	3.6731014133	-2.5437427189	-2.2341139215
H	2.8320439326	-2.4633340207	-0.9775797617
H	5.3520690627	-1.0215948028	-2.0457135578
H	4.2881966277	-0.7121320465	-3.0463591522

Table S4: MP2 OPTIMISED COORDINATES of Water Chloride CLUSTER FOR **Complex 2**

Atom	X	Y	Z
CL	0.	0.	0.
CL	0.	0.	5.3747492
CL	5.3535369682	0.	-0.4770521352
O	2.7737220108	-1.4714541557	0.4391742543
O	-0.6836312771	-1.4714541116	2.6509553766
O	0.0635105247	-2.712659918	-1.7982200989
O	1.7854859558	-2.7126598798	5.1518831776
O	1.6921685598	-3.0770929341	2.4588826063
O	2.7541651066	-3.0770929068	-1.9442960479
O	4.6699056863	-1.4714541116	-3.2008459523
H	2.0087406361	-0.9067918666	0.3501511224
H	3.5482993884	-0.9277798133	0.3407051771
H	-0.5232149529	-0.9534258486	3.4327858276
H	-0.5577870458	-0.9046759819	1.8984389803
H	0.9870952437	-2.8249644288	-1.9648692153
H	-0.0318920881	-1.9445000227	-1.2467536014
H	1.873847369	-2.8393273845	4.2141119716
H	1.2910512322	-1.9102441977	5.270563117
H	2.2107928415	-2.5847486765	1.8332590205
H	0.8331561231	-2.6604070441	2.4590257901
H	3.4966295894	-2.7251609559	-2.4124979376
H	2.7812524041	-2.6717999504	-1.078503426
H	5.0658916026	-1.1210961901	-2.3989510176
H	3.9259776779	-0.9042756868	-3.33534292

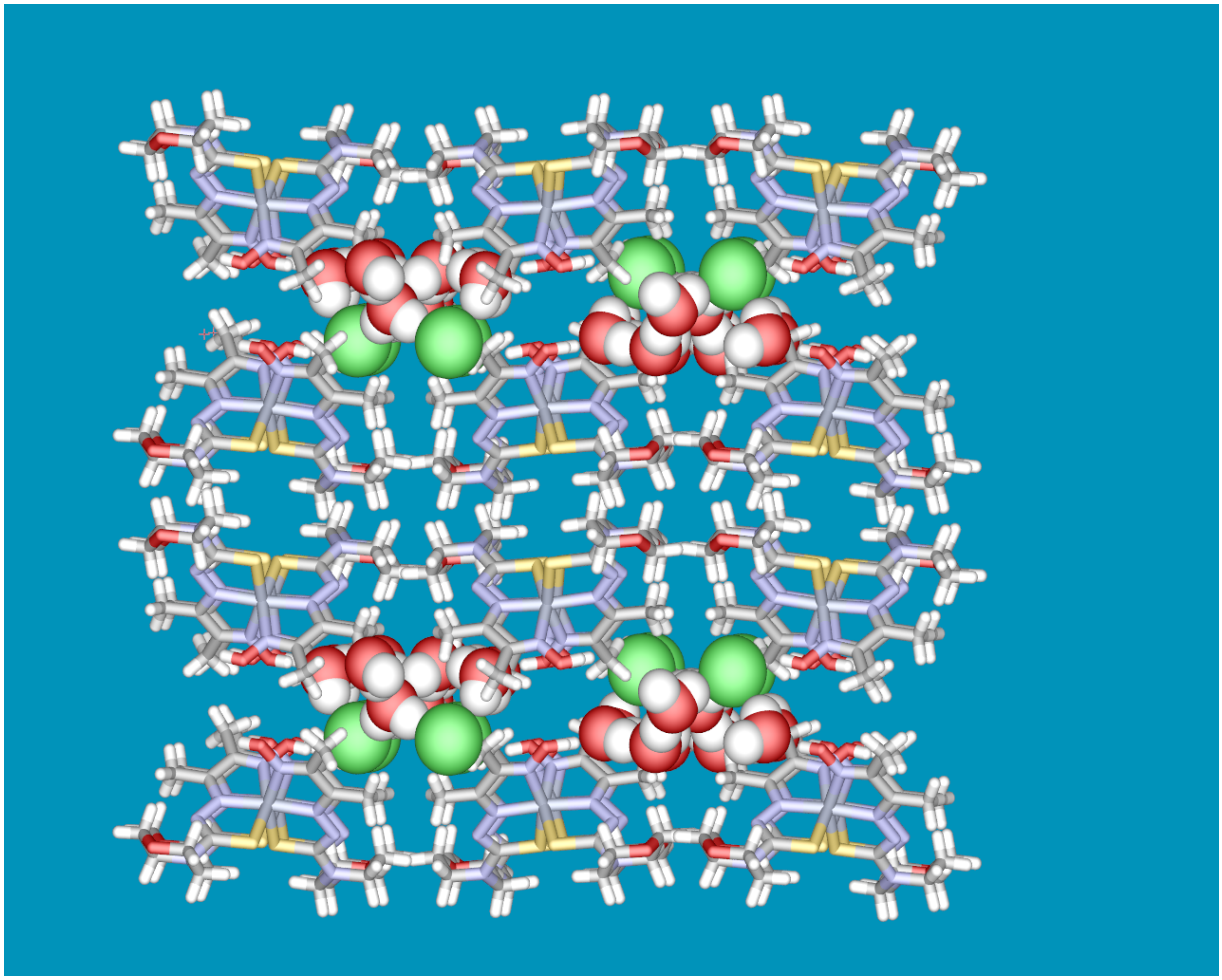

Figure S1: The supramolecular channels are filled up by water-chloride cluster

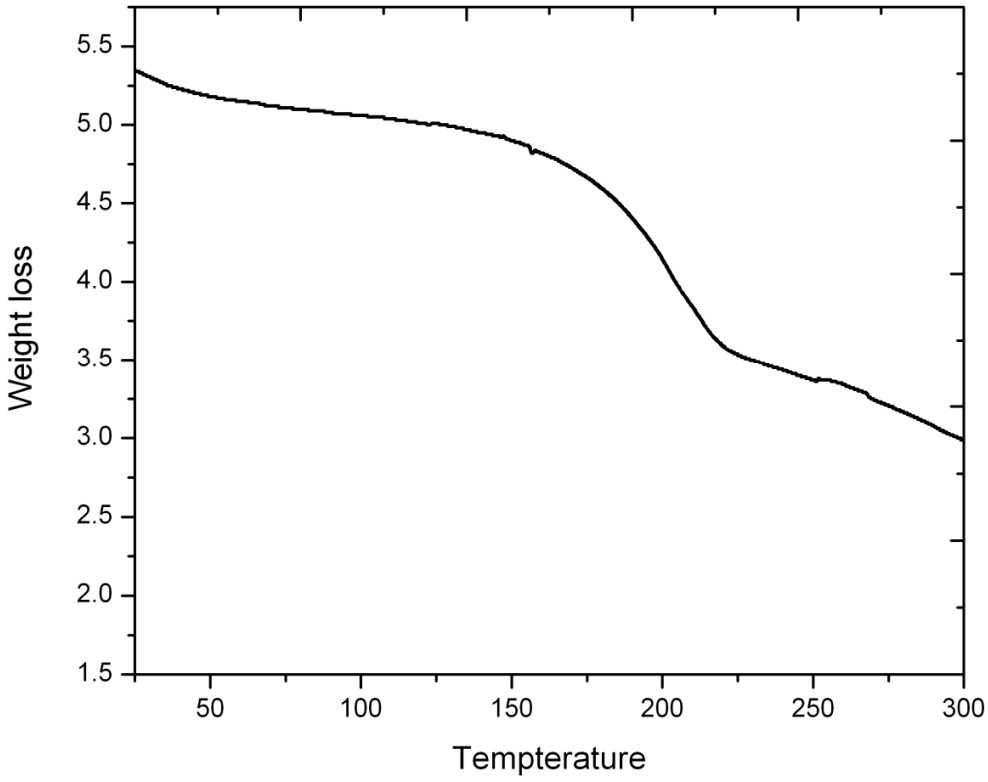

Figure S2: The thermal plot (weight change vs temp) of **complex1**

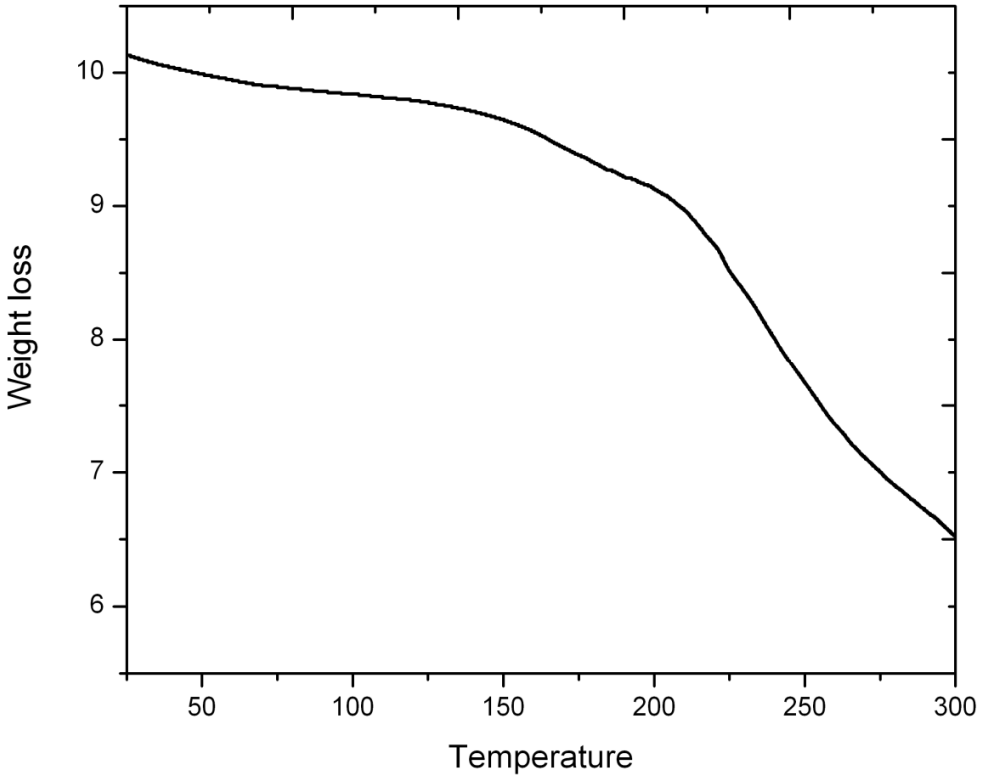

Figure S3: The thermal plot (weight change vs temp) of **complex 2**

(At higher temperature both compounds explodes due to unknown cause.)

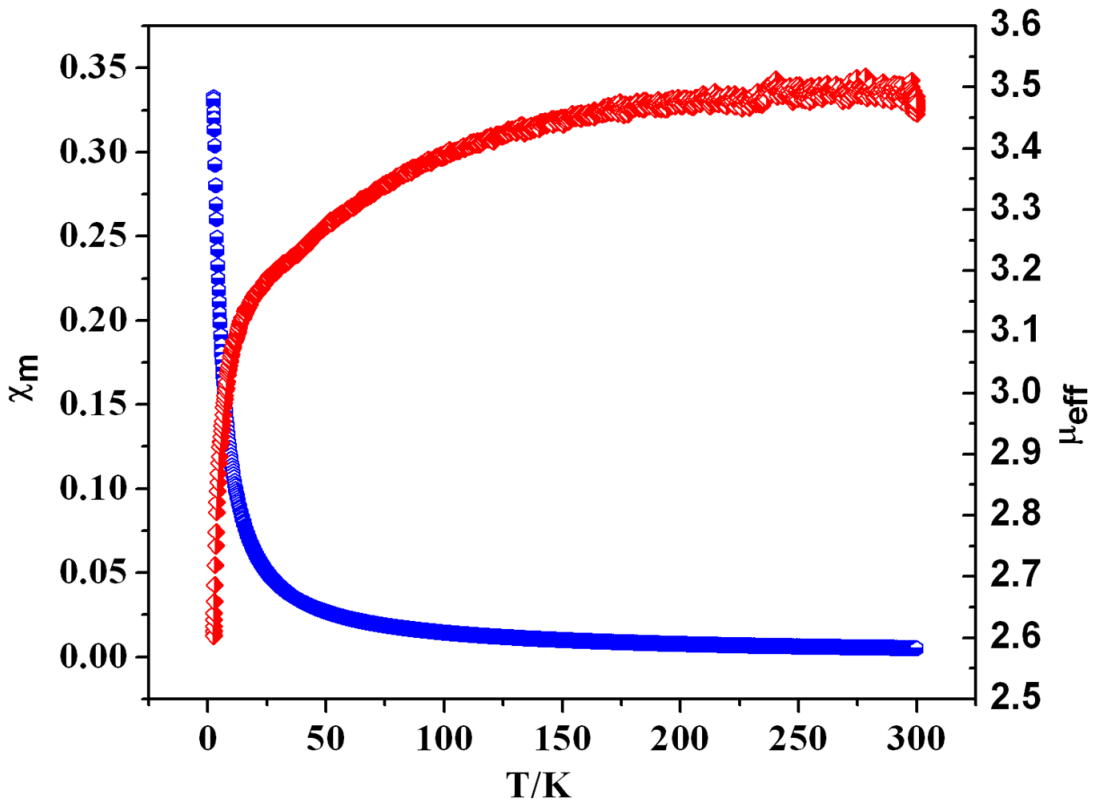

Figure S4: Temperature dependence of χ_M vs T and μ_{eff} vs T for **complex 2**

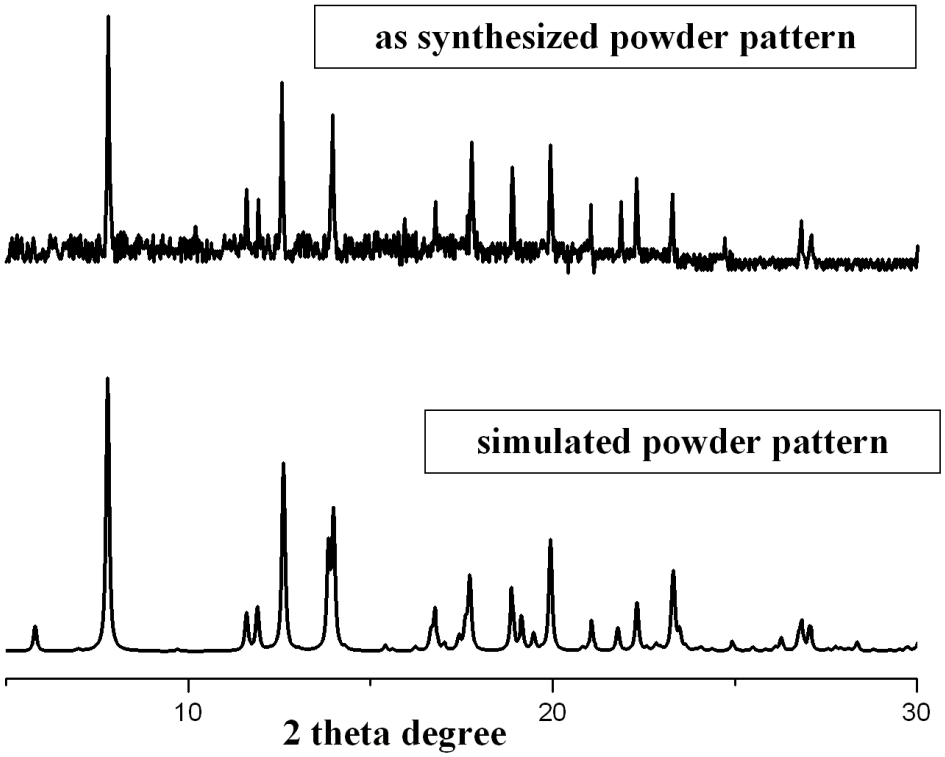

Figure S5: Powder XRD pattern at room temperature of **complex 2**