A facile synthesis, crystal structure and bioactivity evaluation of two novel barium complexes based on 2,4,6-trichlorophenoxyacetic acid and *o*-ferrocenylcarbonyl benzoic acid

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Table S1. Crystallographic data and refinement details for **1** and **2**

Complexes	**1**	**2**
Empirical formula	$BaC_{16}H_{16}Cl_6O_{10}$	$BaC_{36}H_{54}Fe_2O_{20}$
Formula weight	718.33	1055.83
Temperature (K)	298(2)	293(2) (2)
Crystal system	Orthorhombic	Triclinic
space group	*Pbcm*	*P-1*
a, Å	4.2229(6)	9.3623(6)
b, Å	13.994(2)	11.8133(15)
c, Å	42.276(6)	20.503(2)
α (°)	90.00	77.7340(10)
β (°)	96.00	89.018(2)
γ (°)	90.00	89.116(2)
Volume (Å ^{3})	2498.3(6)	2215.3(4)
Z	4	2
Calculated density ($mg \cdot m^{-3}$)	1.910	1.583
Absorption coefficient (mm^{-1})	2.279	1.600
F (000)	1400	1076
Crystal size (mm)	0.30 x 0.30 x 0.30	0.40 x 0.39 x 0.15
Index range	-5<=h<=5 -17<=k<=18 -54<=l<=50	-11<=h<=11 -13<=k<=14 -23<=l<=24
Reflections collected / unique	15055 / 2924	7745 / 7745
R (int)	0.0489	0.0000
Completeness (%)	99.9	99.2
Data / restraints / parameters	2924 / 0 / 154	7745 / 0 / 533
Goodness-of-fit on F^2	1.178	1.039
Final *R* indices [I>2sigma(I)]	R_1 = 0.0589 wR_2 = 0.1655	R_1 = 0.1079 wR_2 = 0.2672
R indices (all data)	R_1 = 0.0652 wR_2 = 0.1764	R_1 = 0.1731 wR_2 = 0.3393

Largest diff .peak and hole (eÅ^{-3})	2.066 and -4.902	1.536 and -1.339

Table S2. Selected bond lengths (Å) and angles (°) for **1** and **2**

	1
Ba(1)-O(3W)	2.718(7)
Ba(1)-O(2W)	2.723(8)
Ba(1)-O(3)	2.761(5)
Ba(1)-O(3)A	2.761(5)
Ba(1)-O(3W)B	2.792(7)
Ba(1)-O(1W)B	2.876(6)
Ba(1)-O(1W)C	2.876(6)
Ba(1)-O(1W)A	2.953(6)
Ba(1)-O(1W)	2.953(6)
O(3W)-Ba(1)-O(2W)	127.5(2)
O(3W)-Ba(1)-O(3)	74.61(17)
O(2W)-Ba(1)-O(3)	120.18(13)
O(3W)-Ba(1)-O(3W)B	100.1(2)
O(2W)-Ba(1)-O(3W)B	132.4(2)
O(3)-Ba(1)-O(3W)B	67.85(15)
O(3W)B-Ba(1)-O(1W)B	70.21(16)
O(3W)-Ba(1)-O(1W)A	70.03(15)
O(1W)C-Ba(1)-O(1W)A	92.84(16)
O(3W)-Ba(1)-O(1W)	70.03(15)
O(2W)-Ba(1)-O(1W)	68.31(18)
O(3)-Ba(1)-O(1W)	73.11(17)
O(1W)B-Ba(1)-O(1W)	92.84(16)
	2
Ba(1)-O(11)	2.69(2)
Ba(1)-O(14)	2.759(17)
Ba(1)-O(8)	2.760(13)
Ba(1)-O(12)	2.77(3)
Ba(1)-O(13)	2.79(2)
Ba(1)-O(9)	2.811(15)
Ba(1)-O(10)	2.822(14)
Ba(1)-O(7)	2.890(11)
O(11)-Ba(1)-O(14)	75.7(6)
O(11)-Ba(1)-O(8)	72.9(6)
O(14)-Ba(1)-O(8)	134.3(6)
O(11)-Ba(1)-O(12)	138.6(7)
O(14)-Ba(1)-O(12)	134.2(7)
O(8)-Ba(1)-O(12)	65.7(6)
O(11)-Ba(1)-O(13)	139.6(8)
O(14)-Ba(1)-O(13)	128.7(7)
O(8)-Ba(1)-O(13)	96.4(7)
O(12)-Ba(1)-O(13)	51.4(8)
O(11)-Ba(1)-O(9)	67.7(7)
O(14)-Ba(1)-O(9)	126.6(6)
O(8)-Ba(1)-O(9)	68.6(4)
O(12)-Ba(1)-O(9)	98.2(7)
O(13)-Ba(1)-O(9)	72.1(6)
O(11)-Ba(1)-O(10)	92.0(6)
O(14)-Ba(1)-O(10)	67.9(5)

Symmetry transformations used to generate equivalent atoms:

[1] A x, y, -z+1/2, B x-1, y, z, C x-1, y, -z, D x+1, y, z; [2] A -x+2, -y+1, -z+1

Table S3. Allelopathic Effects Raphanus sativus of ligand and complex **1** and **2**

Compound	Germination rate				Shoot elongation（RI）				Root elongation（RI）			
	50	100	150	200	50	100	150	200	50	100	150	200
HTCPA	0.61	0.89	0.50	0.45	-0.51	-0.54	-0.60	-0.77	-0.36	-0.58	-0.85	-0.88
1	0.55	0.72	0.78	0.72	-0.46	-0.50	-0.51	-0.56	-0.16	-0.39	-0.45	-0.48
***o*-$OOCC_6H_4$-COFc**	0.72	0.61	0.66	0.83	-0.25	-0.31	-0.33	-0.52	-0.46	-0.51	-0.63	-0.67
2	0.39	0.56	0.83	0.61	-0.17	-0.29	-0.31	-0.33	-0.35	-0.51	-0.53	-0.57
gp	0.56	0.78	0.72	0.67	-0.34	-0.46	-0.58	-0.90	-0.38	-0.78	-0.83	-0.95
ck	0.44	0.89	0.50	0.44								

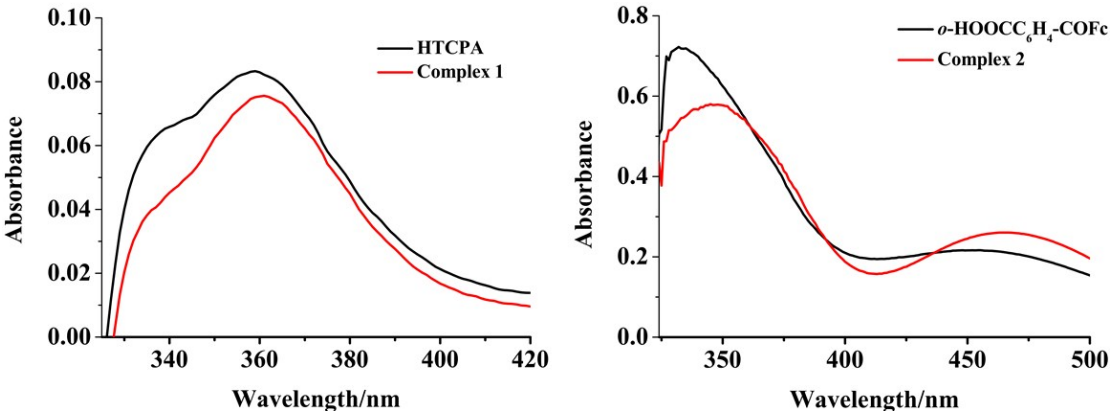

Fig. S1 UV-vis spectra of ligands and complexes.

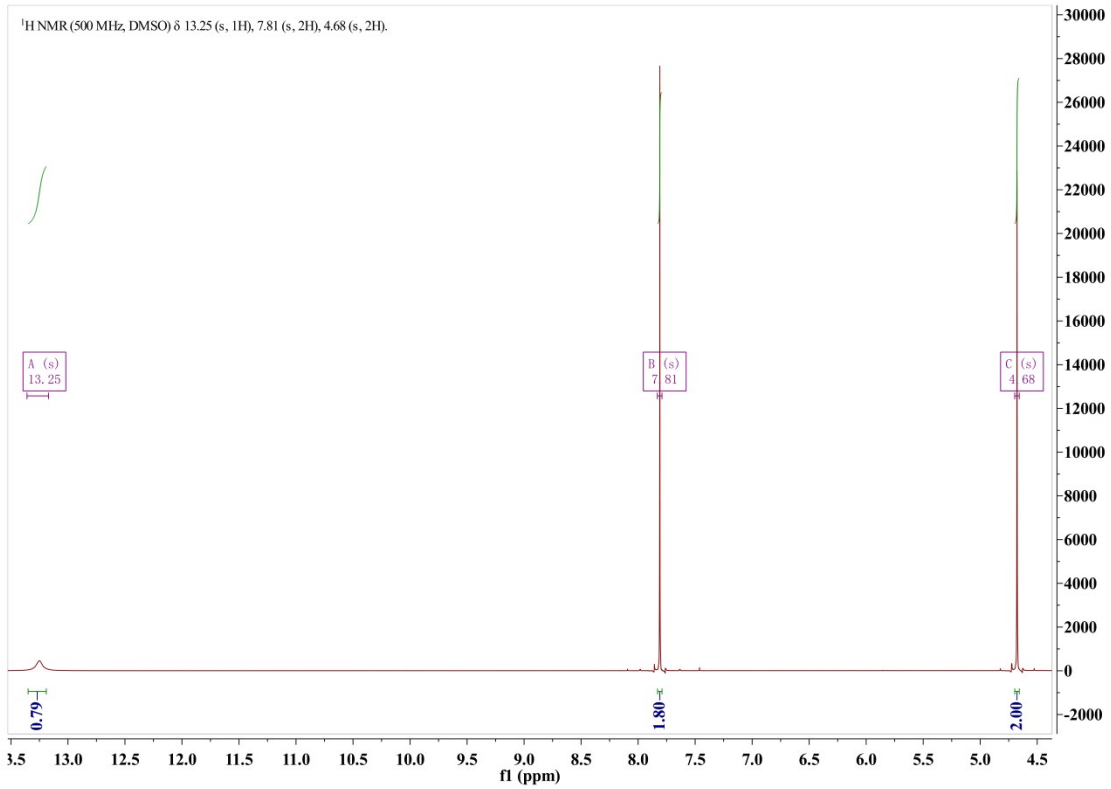

Fig. S2 ¹HNMR spectra of **HTCPA**.

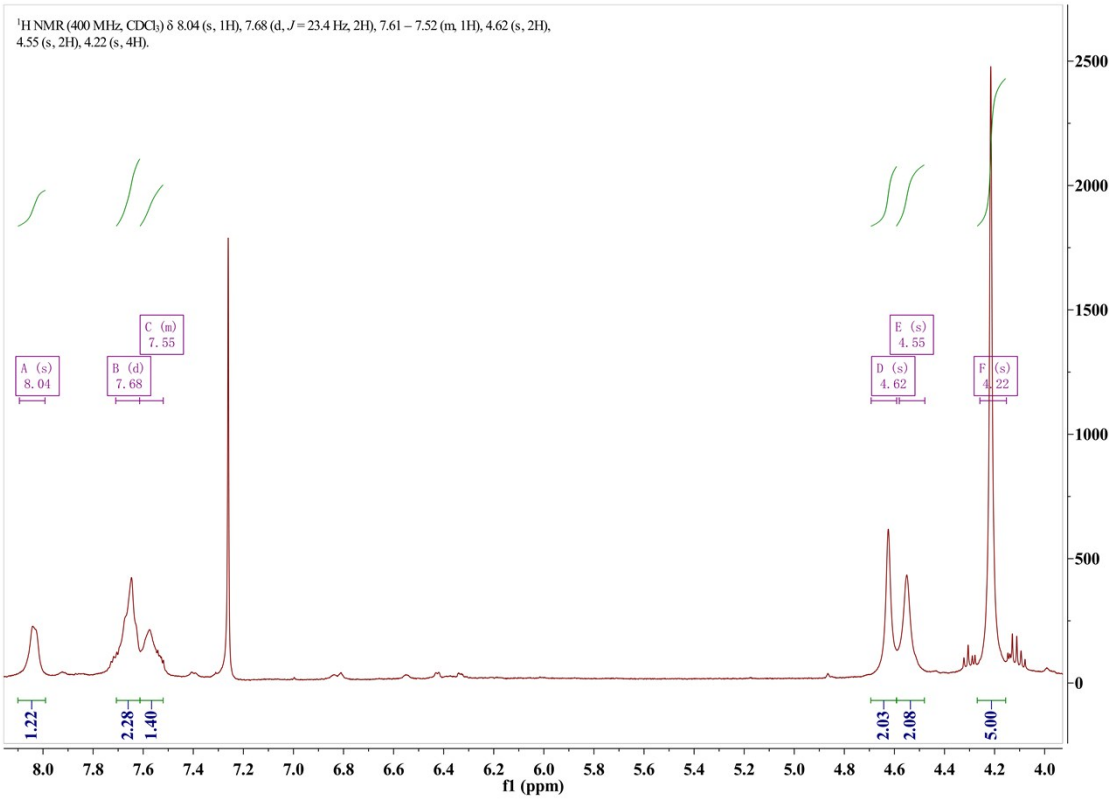

Fig. S3 ¹HNMR spectra of ***o*-HOOCC$_6$H$_4$-COFc**.

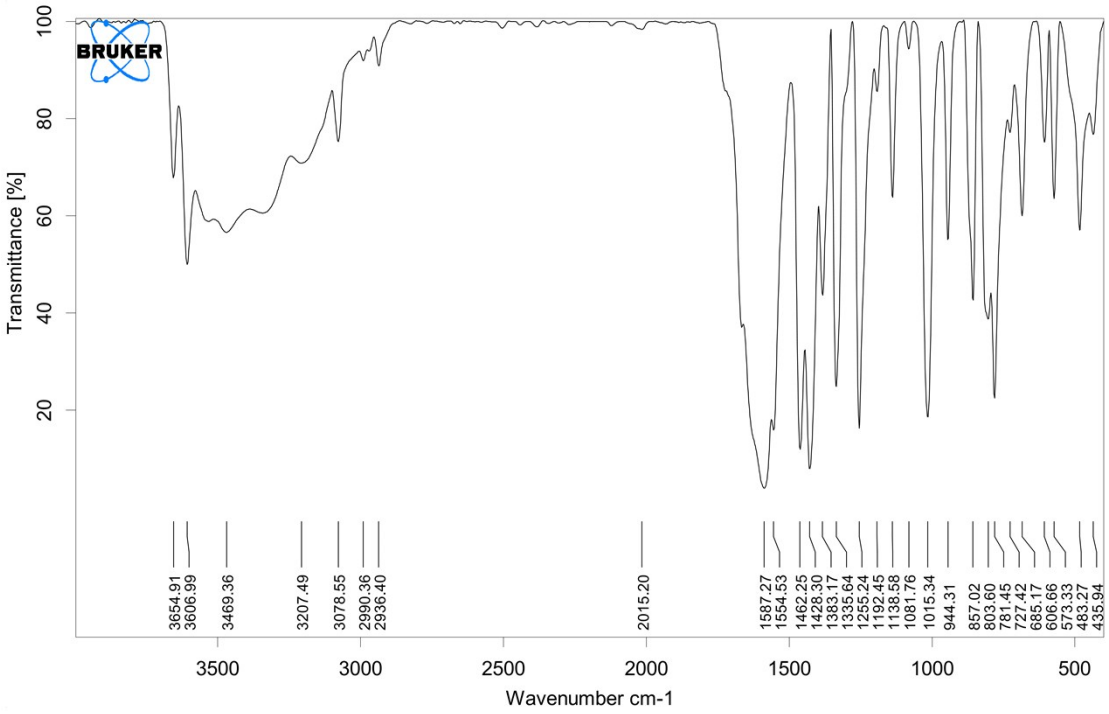

Fig. S4 IR spectra of complexes **1**.

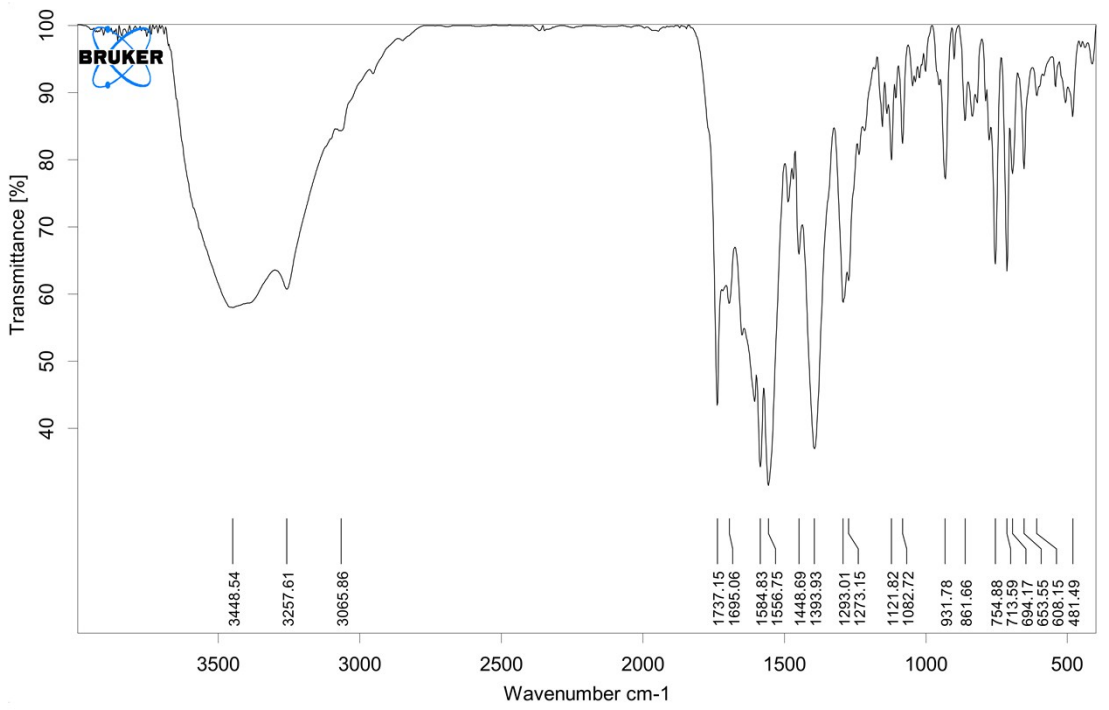

Fig. S5 IR spectra of complexes **2**.

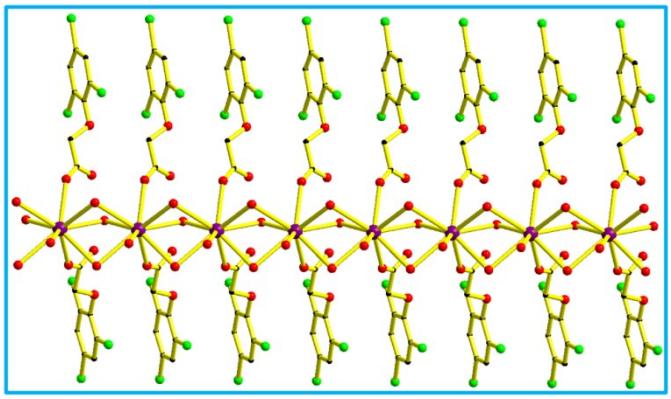

Fig. S6 The 1D chain of complex **1**.

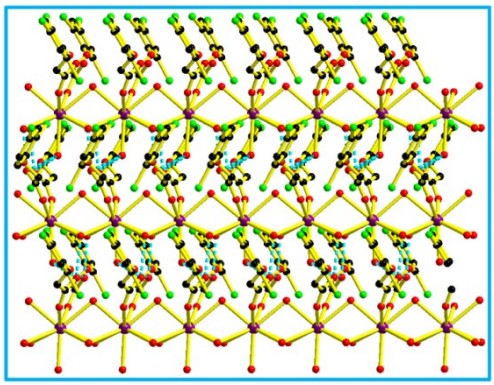

Fig. S7 The 2D layer of complex **1**.

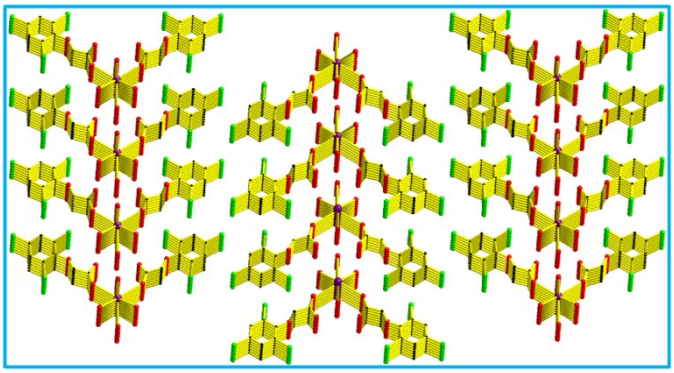

Fig. S8 The 3D network of complex **1**.

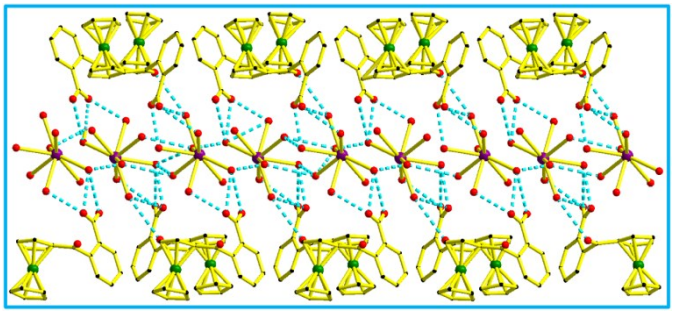

Fig. S9 The 1D chain of complex **2**.

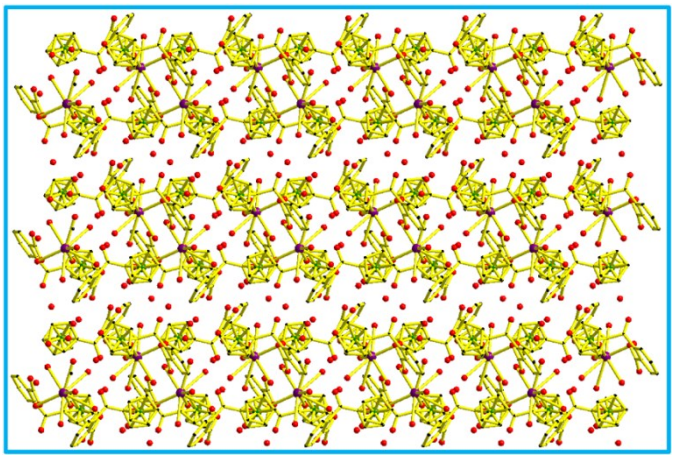

Fig. S10 The 2D layer of complex **2**.

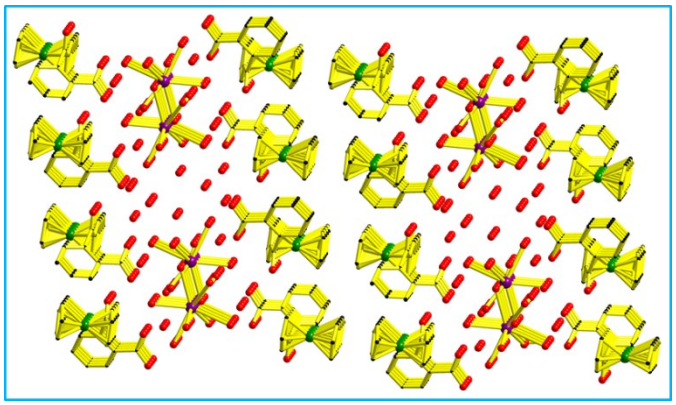

Fig. S11 The 3D network of complex **2**.

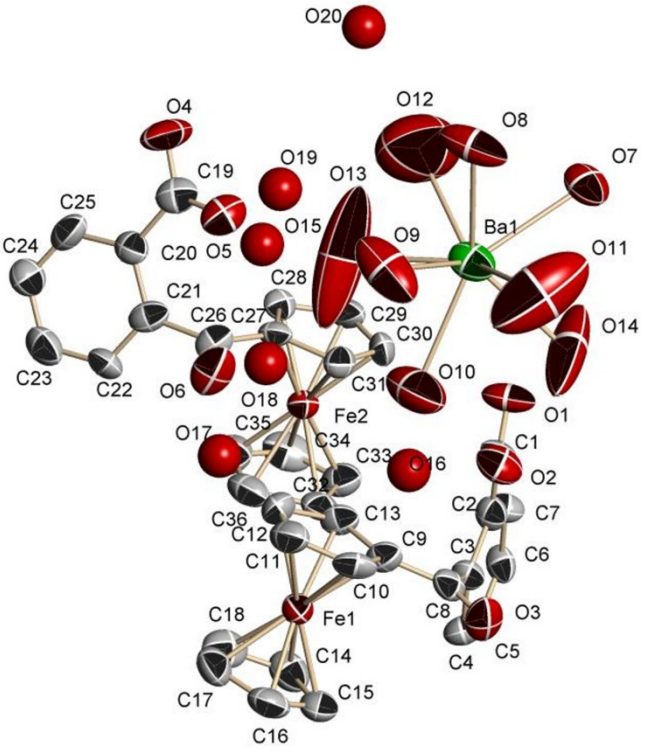

Fig. S12 The ORTEP-style diagram of complex **1**.

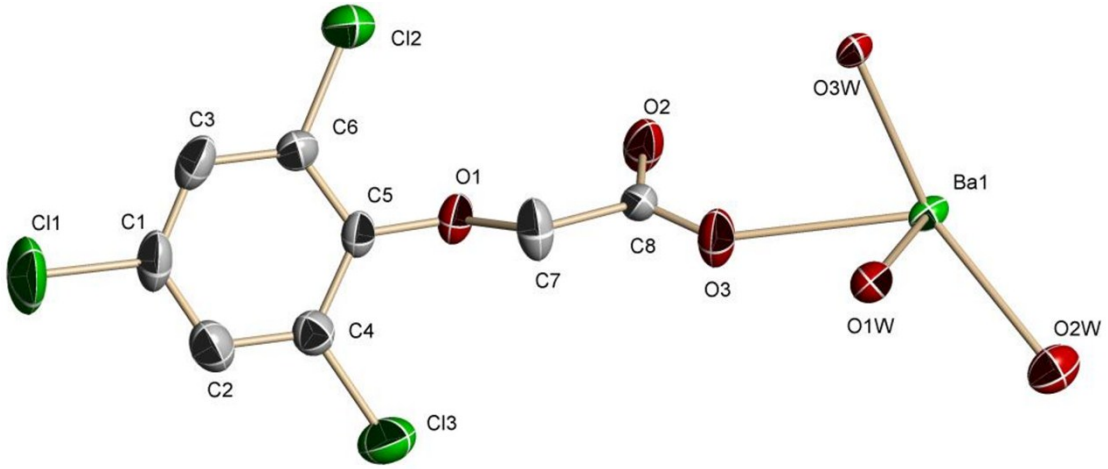

Fig. S13 The ORTEP-style diagram of complex **2**.