## 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

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

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

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

Fig. S2 <sup>1</sup>HNMR spectra of HTCPA.

Fig. S3 <sup>1</sup>HNMR spectra of *o*-HOOCC<sub>6</sub>H<sub>4</sub>-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.

Complexes	1	2		
Empirical formula	$BaC_{16}H_{16}Cl_6O_{10}$	BaC <sub>36</sub> H <sub>54</sub> Fe <sub>2</sub> O <sub>20</sub>		
Formula weight	718.33	1055.83		
Temperature (K)	298(2)	293(2) (2)		
Crystal system	Orthorhombic	Triclinic		
space group	Pbcm	P-1		
<i>a</i> , Å	4.2229(6)	9.3623(6)		
b, Å	13.994(2)	11.8133(15)		
<i>c</i> , 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 <sup>3</sup> )	2498.3(6)	2215.3(4)		
Ζ	4	2		
Calculated density (mg·m <sup>-3</sup> )	1.910	1.583		
Absorption coefficient (mm <sup>-1</sup> )	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		
	-5<=h<=5	-11<=h<=11		
	-17<=k<=18	-13<=k<=14		
Index range	-54<=l<=50	-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 <i>R</i> indices [I>2sigma(I)]	$R_1 = 0.0589$	$R_1 = 0.1079$		
L - 6 - (7)	$wR_2 = 0.1655$	$wR_2 = 0.2672$		
R indices (all data)	$R_1 = 0.0652$ $wR_2 = 0.1764$	$R_1 = 0.1731$ $wR_2 = 0.3393$		

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

Largest diff .peak and hole (eÅ-

2.066 and -4.902 1.536 and -1.339

3)

I     Ba(1)-Q(3W)   2.718(7)     Ba(1)-Q(2W)   2.723(8)     Ba(1)-Q(3)   2.761(5)     Ba(1)-Q(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)A   2.953(6)     O(3W)-Ba(1)-O(2W)   127.5(2)     O(3W)-Ba(1)-O(3W)B   100.1(2)     O(2W)-Ba(1)-O(3W)B   100.1(2)     O(2W)-Ba(1)-O(3W)B   132.4(2)     O(3W)-Ba(1)-O(3W)B   74.51(17)     O(2W)-Ba(1)-O(3W)B   70.21(16)     O(3W)-Ba(1)-O(1W)A   70.03(15)     O(1W)C-Ba(1)-O(1W)A   70.33(15)     O(2W)-Ba(1)-O(1W)A   70.31(17)     O(3W)-Ba(1)-O(1W)A   70.31(17)     O(1W)C-Ba(1)-O(1W)A   70.31(15)     O(2W)-Ba(1)-O(1W)   73.11(17)     O(1W)C-Ba(1)-O(1W)   75.91(7)     Ba(1)-O(11)   2.69(2)     Ba(1)-O(11)   2.69(2)     Ba(1)-O(12)   2.77(3)     Ba(1)-O(13)   2.890(11)     O(11)-Ba(1)-O(18) <td< th=""><th></th><th></th></td<>			
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O(3W)-Ba(1)-O(3W)B $100.1(2)$ $O(2W)-Ba(1)-O(3W)B$ $132.4(2)$ $O(3)-Ba(1)-O(3W)B$ $67.85(15)$ $O(3W)-Ba(1)-O(1W)A$ $70.21(16)$ $O(3W)-Ba(1)-O(1W)A$ $70.3(15)$ $O(1W)C-Ba(1)-O(1W)A$ $92.84(16)$ $O(3W)-Ba(1)-O(1W)$ $68.31(18)$ $O(3)-Ba(1)-O(1W)$ $68.31(18)$ $O(3)-Ba(1)-O(1W)$ $73.11(17)$ $O(1W)B-Ba(1)-O(1W)$ $92.84(16)$ 2Ba(1)-O(11)2.69(2)Ba(1)-O(14)2.759(17)Ba(1)-O(14)2.77(3)Ba(1)-O(12)2.811(15)Ba(1)-O(1)2.880(11)O(10)2.822(14)Ba(1)-O(10)2.822(14)Ba(1)-O(14)7.76(6)O(11)-Ba(1)-O(14)7.76(6)O(14)-Ba(1)-O(12)138.6(7)O(14)-Ba(1)-O(12)134.2(7)O(8)-Ba(1)-O(13)139.6(8)O(14)-Ba(1)-O(13)139.6(8)O(14)-Ba(1)-O(13)139.6(8)O(14)-Ba(1)-O(13)139.6(8)O(14)-Ba(1)-O(13)139.6(8)O(14)-Ba(1)-O(13)139.6(8)O(14)-Ba(1)-O(13) </td <td>O(2W)-Ba(1)-O(3)</td> <td>120.18(13)</td>	O(2W)-Ba(1)-O(3)	120.18(13)	
O(2W)-Ba(1)-O(3W)B $132.4(2)$ $O(3)-Ba(1)-O(3W)B$ $67.85(15)$ $O(3W)B-Ba(1)-O(1W)B$ $70.21(16)$ $O(3W)-Ba(1)-O(1W)A$ $70.03(15)$ $O(1W)C-Ba(1)-O(1W)A$ $92.84(16)$ $O(3W)-Ba(1)-O(1W)$ $70.03(15)$ $O(2W)-Ba(1)-O(1W)$ $68.31(18)$ $O(3)-Ba(1)-O(1W)$ $73.11(17)$ $O(1W)B-Ba(1)-O(1W)$ $73.11(17)$ $O(1W)B-Ba(1)-O(1W)$ $92.84(16)$ <b>2</b> Ba(1)-O(11)2.69(2)Ba(1)-O(14)2.759(17)Ba(1)-O(14)2.77(3)Ba(1)-O(12)2.811(15)Ba(1)-O(13)2.811(15)Ba(1)-O(10)2.822(14)Ba(1)-O(10)2.822(14)Ba(1)-O(10)2.822(14)Ba(1)-O(14)7.7(6)O(11)-Ba(1)-O(14)7.7(6)O(14)-Ba(1)-O(12)138.6(7)O(14)-Ba(1)-O(12)138.6(7)O(14)-Ba(1)-O(13)139.6(8)O(14)-Ba(1)-O(13)139.6(8)O(14)-Ba(1)-O(13)139.6(8)O(14)-Ba(1)-O(13)139.6(8)O(14)-Ba(1)-O(13)139.6(8)O(14)-Ba(1)-O(13)	O(3W)-Ba(1)-O(3W)B	100.1(2)	
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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)- $O(1W)$ 68.31(18) $O(2W)$ -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) <b>2</b> Ba(1)- $O(11)$ 2.69(2)Ba(1)- $O(14)$ 2.759(17)Ba(1)- $O(14)$ 2.77(3)Ba(1)- $O(12)$ 2.77(3)Ba(1)- $O(13)$ 2.822(14)Ba(1)- $O(10)$ 2.822(14)Ba(1)- $O(12)$ 1.846(7)O(11)-Ba(1)- $O(12)$ 1.38.6(7)O(14)-Ba(1)- $O(13)$ 1.39.6(8)O(14)-Ba(1)- $O(13)$ 1.39.6(8)O(14)-Ba(1)- $O(13)$ 1.39.6(8)O(14)-Ba(1)- $O(13)$ 1.39.6(8)O(14)-Ba(1)- $O(13)$ 1.39.6(8)	O(3W)B-Ba(1)-O(1W)B	70.21(16)	
$\begin{array}{llllllllllllllllllllllllllllllllllll$	O(3W)-Ba(1)-O(1W)A	70.03(15)	
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Ba(1)-O(9) $2.811(15)$ $Ba(1)-O(10)$ $2.822(14)$ $Ba(1)-O(7)$ $2.890(11)$ $O(11)-Ba(1)-O(14)$ $75.7(6)$ $O(11)-Ba(1)-O(18)$ $72.9(6)$ $O(14)-Ba(1)-O(8)$ $134.3(6)$ $O(11)-Ba(1)-O(12)$ $138.6(7)$ $O(14)-Ba(1)-O(12)$ $134.2(7)$ $O(8)-Ba(1)-O(12)$ $65.7(6)$ $O(11)-Ba(1)-O(13)$ $139.6(8)$ $O(14)-Ba(1)-O(13)$ $128.7(7)$ $O(8)-Ba(1)-O(13)$ $96.4(7)$ $O(12)-Ba(1)-O(13)$ $51.4(8)$	Ba(1)-O(13)	2.79(2)	
Ba(1)-O(10) $2.822(14)$ $Ba(1)-O(7)$ $2.890(11)$ $O(11)-Ba(1)-O(14)$ $75.7(6)$ $O(11)-Ba(1)-O(8)$ $72.9(6)$ $O(14)-Ba(1)-O(8)$ $134.3(6)$ $O(14)-Ba(1)-O(12)$ $138.6(7)$ $O(14)-Ba(1)-O(12)$ $134.2(7)$ $O(8)-Ba(1)-O(12)$ $65.7(6)$ $O(11)-Ba(1)-O(13)$ $139.6(8)$ $O(14)-Ba(1)-O(13)$ $128.7(7)$ $O(8)-Ba(1)-O(13)$ $96.4(7)$ $O(12)-Ba(1)-O(13)$ $51.4(8)$	Ba(1)-O(9)	2.811(15)	
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)	Ba(1)-O(10)	2.822(14)	
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)	Ba(1)-O(7)	2.890(11)	
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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(8)	72.9(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(14)-Ba(1)-O(8)	134.3(6)	
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(12)	138.6(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(14)-Ba(1)-O(12)	134.2(7)	
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(8)-Ba(1)-O(12)	65.7(6)	
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(13)	139.6(8)	
$\begin{array}{c} O(8)-Ba(1)-O(13) \\ O(12)-Ba(1)-O(13) \\ O(12)-O(13) \\ O(12$	O(14)-Ba(1)-O(13)	128.7(7)	
O(12)-Ba(1)-O(13) 51 4(8)	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(11)-Ba(1)-O(9)	67.7(7)	
O(14)-Ba(1)-O(9) 126 6(6)	O(14)-Ba(1)-O(9)	126.6(6)	
O(8)-Ba(1)- $O(9)$ 68 6(4)	O(8)-Ba(1)-O(9)	68 6(4)	
O(12)-Ba(1)-O(9) 98 2(7)	O(12)-Ba(1)-O(9)	98 2(7)	
O(13)-Ba(1)-O(9) 72 1(6)	O(13)-Ba(1)-O(9)	72.1(6)	
O(11)-Ba(1)-O(10) 92 0(6)	O(11)-Ba(1)-O(10)	92.0(6)	
O(14)-Ba(1)-O(10) 67 9(5)	O(14)-Ba(1)-O(10)	67.9(5)	

Table S2. Selected bond lengths (Å) and angles (°) for 1 and 2  $\,$ 

Symmetry transformations used to generate equivalent atoms:

$1 \Delta x v - z + 1/2 B x - 1 v z C x - 1 v - z D x + 1 v z - 2 \Delta - x + 2 - v + 1 - z + 1$					
	$^{1}$ A x v $-z+1/2$	Bx-1 vz	Cx-1 v - z D x-	+1 v z <sup>·2</sup> A -x-	+2 -v+1 -z+1

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

Gamma	Germination rate				Shoot elongation (RI)			Root elongation (RI)				
Compound	50	100	150	200	50	100	150	200	50	100	150	200
НТСРА	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-OOCC6H4-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. 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.