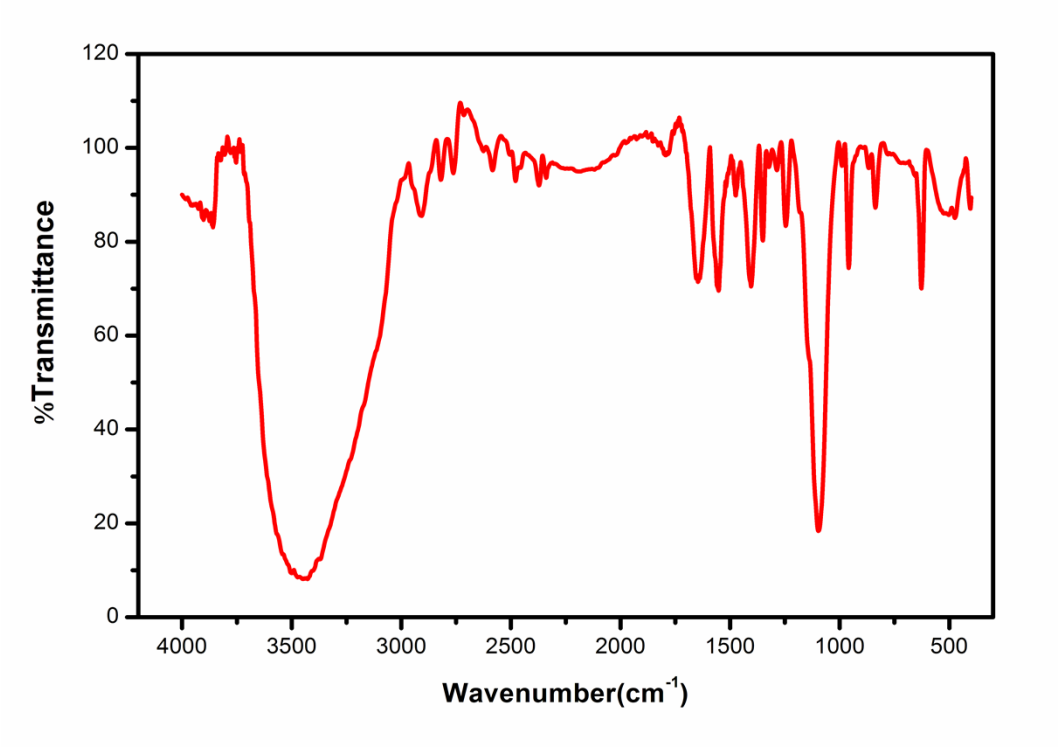

Fig.S1 The IR spectrum for compound 1

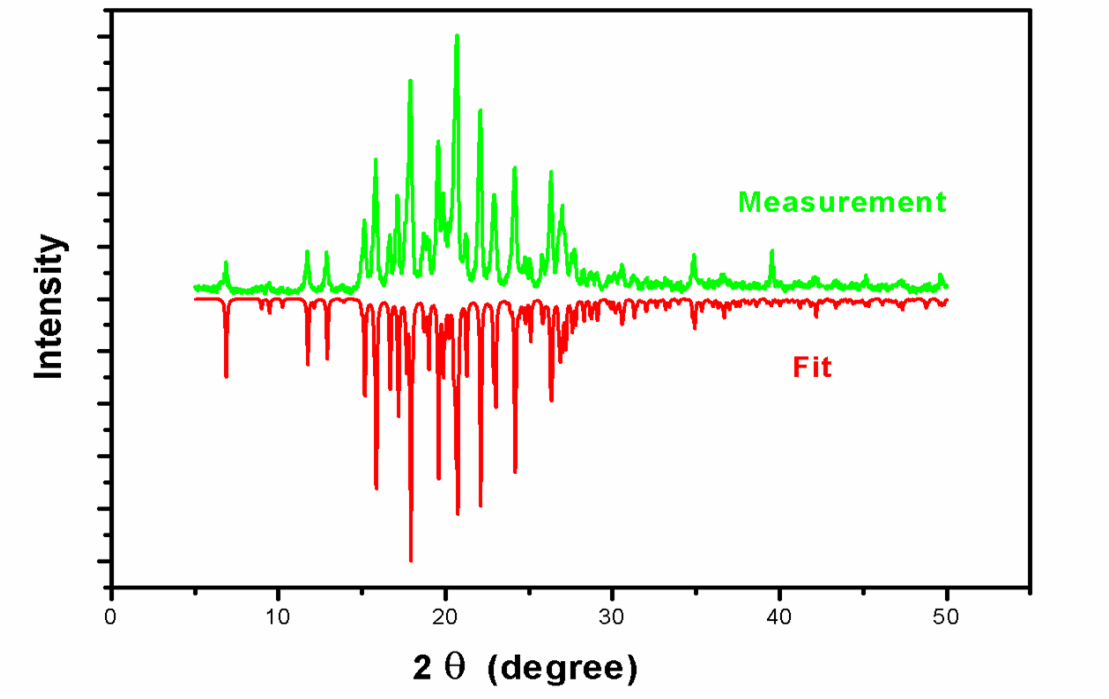

Fig.S2 The powder X-ray diffraction (PXRD) pattern for compound 1

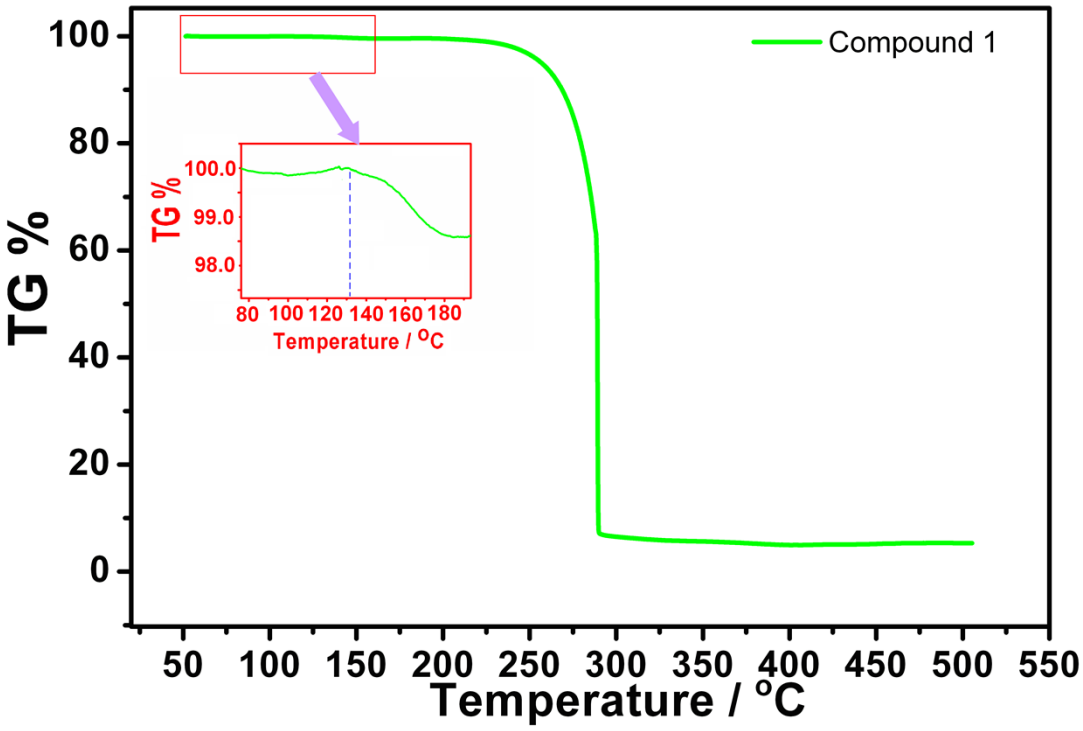

Fig.S3 Thermogravimetric(TG) measurements of compound 1 in N2 atmosphere.

Structure refinement:

The restraints (SIMU, DELU and FREE) were used to improve the quality of the refinements of the two structures.

For 293k: simu o11 cl2 o10, delu o11 cl2 o10, free c11 c11', free c6 c6'.

For 383k: dfix 1.45 cl2 o11, simu cl2 o12 o13 o14 o3 c6 c6' c3, delu o3 c6 c6' c3, free c11 c11', free c6 c6'.

Table S1 Selected structural data for 1under 293K

Bond lengths / Å and bond angles / °			
Cl(1)-O(7)	1.399(4)	Cl(2)-O(11)	1.194(5)
Cl(1)-O(7)#2	1.399(4)	Cl(2)-O(13)	1.255(1)
Cl(1)-O(10)	1.419(7)	Cl(2)-O(13)#1	1.255(1)
Cl(1)-O(9)	1.425(6)	Cl(2)-O(12)	1.361(1)
O(7)-Cl(1)-O(7)#2	110.1(5)	O(11)-Cl(2)-O(13)	118.6(9)
O(7)-Cl(1)-O(10)	109.8(3)	O(11)-Cl(2)-O(13)#1	118.6(9)
O(7)#2-Cl(1)-O(10)	109.8(3)	O(13)-Cl(2)-O(13)#1	109.4(1)
O(7)-Cl(1)-O(9)	109.3(3)	O(11)-Cl(2)-O(12)	97.4(1)
O(7)#2-Cl(1)-O(9)	109.3(3)	O(13)-Cl(2)-O(12)	105.1(1)
O(10)-Cl(1)-O(9)	108.6(5)	O(13)#1-Cl(2)-O(12)	105.1(1)

Hydrogen bonds / Å and °				
D−H···A	d(D−H)	d(H···A)	d(D···A)	<(DHA)
N(1)-H(1C)...O(2)#3	0.91	2.12	2.95(2)	151(2)
N(1)-H(1C)...O(1)#3	0.91	2.23	2.90(1)	130(5)
N(1)-H(1E)...O(3)#3	0.92	2.16	2.88(3)	135(3)
N(1)-H(1E)...O(3)#4	0.92	2.16	2.88(3)	135(3)
N(2)-H(2D)...O(10)#5	0.92	2.19	3.09(1)	168(4)
N(2)-H(2C)...O(12)	0.91	2.55	3.44(3)	163(1)
O(1W)-H(1WB)...O(2)	0.86	2.33	3.10 (2)	151(3)

Symmetry transformations used to generate equivalent atoms: #1 x, -y+1/2, z #2 x, -y+3/2, z ; #3 x, -y+1/2, z+1; #4 x, y, z+1; #5 2-x, -1/2 + y, 1-z

Table S2 Selected structural data for 1 under 368k

Bond lengths / Å and bond angles / °			
Cl(1)-O(7)	1.409(2)	Cl(1)-O(7)#2	1.409 (2)
Cl(1)-O(10)	1.421(3)	Cl(1)-O(9)	1.430(3)
Cl(2)-O(16)	1.385(8)	Cl(2)-O(13)	1.378(4)
Cl(2)-O(13)#1	1.378(4)	Cl(2)-O(14)	1.271(4)
Cl(2)-O(15)#1	1.376(1)	Cl(2)-O(11)	1.432(6)
Cl(2)-O(15)	1.376(1)	Cl(2)-O(12)	1.508(9)
Cl(2)-O(17)	1.444(2)		
O(7)-Cl(1)-O(7)#2	109.79(19)	O(7)-Cl(1)-O(10)	108.8(3)
O(7)#2-Cl(1)-O(10)	108.82(13)	O(7)-Cl(1)-O(9)	109.8(1)
O(7)#2-Cl(1)-O(9)	109.89(10)	O(10)-Cl(1)-O(9)	109.6(2)
O(14)-Cl(2)-O(13)	69.3(2)	O(14)-Cl(2)-O(13)#1	69.3(2) O(13)-
Cl(2)-O(13)#1	111.5(4)	O(14)-Cl(2)-O(15)#1	117.3(5) O(13)-
Cl(2)-O(15)#1	170.2(5)	O(13)#1-Cl(2)-O(15)#1	78.2(5) O(14)-
Cl(2)-O(15)	117.3(5)	O(13)-Cl(2)-O(15)	78.2(5)
O(13)#1-Cl(2)-O(15)	170.2(5)	O(15)#1-Cl(2)-O(15)	92.1(9)
O(14)-Cl(2)-O(16)	178.2(4)	O(13)-Cl(2)-O(16)	111.6(3)
O(13)#1-Cl(2)-O(16)	111.6(3)	O(15)#1-Cl(2)-O(16)	61.6(5)
O(15)-Cl(2)-O(16)	61.6(5)	O(14)-Cl(2)-O(11)	94.9(4)
O(13)-Cl(2)-O(11)	117.8(2)	O(13)#1-Cl(2)-O(11)	117.8(2)
O(15)#1-Cl(2)-O(11)	56.1(5)	O(15)-Cl(2)-O(11)	56.1(5)
O(16)-Cl(2)-O(11)	83.3(5)	O(14)-Cl(2)-O(17)	58.1(7)
O(13)-Cl(2)-O(17)	100.6(4)	O(13)#1-Cl(2)-O(17)	100.6(4)
O(15)#1-Cl(2)-O(17)	78.5(7)	O(15)-Cl(2)-O(17)	78.5(7)
O(16)-Cl(2)-O(17)	120.1(8)	O(11)-Cl(2)-O(17)	36.8(7)
O(14)-Cl(2)-O(12)	136.0(4)	O(13)-Cl(2)-O(12)	87.1(3)
O(13)#1-Cl(2)-O(12)	87.1(3)	O(15)#1-Cl(2)-O(12)	91.9(6)
O(15)-Cl(2)-O(12)	91.9(6)	O(16)-Cl(2)-O(12)	45.9(5)

O(11)-Cl(2)-O(12)	129.1(5)	O(17)-Cl(2)-O(12)	166.0(8)

Hydrogen bonds / Å and °

D−H···A	d(D−H)	d(H···A)	d(D···A)	<(DHA)
N(1)-H(1C)...O(2)#3	0.92	2.14	2.97(2)	151(3)
N(1)-H(1C)...O(1)#3	0.92	2.22	2.90(1)	130(3)
N(1)-H(1E)...O(3)#3	0.92	2.19	2.91(2)	135(2)
O(1W)-H(1WB)...O(2)	0.86	3.07	3.591(1)	121(1)
N(2)-H(2C)...O(15)#1	0.92	2.21	3.05 (3)	151(3)
N(2)-H(2D)...O(10)#5	0.93	2.21	3.13(5)	168(3)
N(2)-H(2C)...O(11)	0.92	2.08	2.86(1)	143(5)
N(2)-H(2C)...O(16)	0.92	2.12	3.01(1)	165(5)

Symmetry transformations used to generate equivalent atoms: #1 x, -y+1/2, z #2 x, -y+3/2, z ; #3 x, -y+1/2, z+1; #4 x, y, z+1; #5 2-x, -1/2 + y, 1-z