Supporting Information

Hydrogen bond synthons affect coordination geometry of d10-metal halide complexes: Synthetic methods, theoretical studies and supramolecular architectures

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Contents

Table S1. Bond lengths (Å) and angles (°) for compound 1

Bond distances	**atom-atom**	**distance**	**atom-atom**	**distance**	**atom-atom**	**distance**
	Hg(1)-Cl(1)	2.3708(9)	C(4)-C(5)	1.378(5)	N(3)-C(10)	1.334(5)
	Hg(1)-N(1)	2.431(3)	C(5)-H(5)	0.9500	N(4)-C(9)	1.335(5)
	Cl(2)-Hg(1)#2	2.9592(9)	C(7)-C(8)	1.383(5)	C(1)-C(2)	1.382(5)
	N(1)-C(1)	1.344(5)	C(9)-C(10)	1.398(5)	C(2)-C(3)	1.382(5)
	N(2)-C (6)	1.357(5)	C(10)-H(10)	0.9500	C(3)-H(3)	0.9500
	N(2)-H(2N)	0.83(4)	Hg(1)-Cl(2)	2.3774(9)	C(4)-H(4)	0.9500
	N(3)-C(7)	1.337(5)	Hg(1)-Cl(2)#1	2.9592(9)	C(6)-C(7)	1.508(5)
	N(4)-C(8)	1.337(5)	O(1)-C(6)	1.224(4)	C(8)-H(8)	0.9500
	C(1)-H(1)	0.9500	N(1)-C(5)	1.345(5)	C(9)-H(9)	0.9500
	C(3)-C(4)	1.389(5)	N(2)-C(2)	1.415(5)		
Bond angles	**atom-atom-atom**	**angle**	**atom-atom-atom**	**angle**	**atom-atom-atom**	
	Cl(1)-Hg(1)-Cl(2)	167.26(3)	O(1)-C(6)-N(2)	124.4(4)	N(1)-C(1)-C(2)	122.5(3)
	Cl(2)-Hg(1)-N(1)	96.42(8)	N(2)-C(6)-C(7)	115.9(3)	C(2)-C(1)-H(1)	118.7
	Cl(2)-Hg(1)-Cl(2)#1	90.41(3)	N(3)-C(7)-C(6)	119.2(3)	C(1)-C(2)-N(2)	117.7(3)
	Hg(1)-Cl(2)-Hg(1)#2	90.41(3)	N(4)-C(8)-C(7)	122.2(3)	C(2)-C(3)-C(4)	118.1(3)
	C(1)-N(1)-Hg(1)	121.9(2)	C(7)-C(8)-H(8)	118.9	C(4)-C(3)-H(3)	120.9
	C(6)-N(2)-C(2)	125.4(3)	N(4)-C(9)-H(9)	118.9	C(5)-C(4)-H(4)	120.2
	C(2)-N(2)-H(2N)	121(3)	N(3)-C(10)-C(9)	121.9(3)	N(1)-C(5)-C(4)	122.4(3)
	C(9)-N(4)-C(8)	115.6(3)	C(9)-C(10)-H(10)	119.0	C(4)-C(5)-H(5)	118.8
	N(1)-C(1)-H(1)	118.7	Cl(1)-Hg(1)-N(1)	96.31(8)	O(1)-C(6)-C(7)	119.7(3)
	C(1)-C(2)-C(3)	119.4(3)	Cl(1)-Hg(1)-Cl(2)#1	89.54(3)	N(3)-C(7)-C(8)	122.5(3)
	C(3)-C(2)-N(2)	122.8(3)	N(1)-Hg(1)-Cl(2)#1	88.00(7)	C(8)-C(7)-C(6)	118.3(3)
	C(2)-C(3)-H(3)	120.9	C(1)-N(1)-C(5)	118.0(3)	N(4)-C(8)-H(8)	118.9

	C(5)-C(4)-C(3)	119.5(4)	C(5)-N(1)-Hg(1)	120.1(2)	N(4)-C(9)-C(10)	122.2(3)
	C(3)-C(4)-H(4)	120.2	C(6)-N(2)-H(2N)	113(3)	C(10)-C(9)-H(9)	118.9
	N(1)-C(5)-H(5)	118.8	C(10)-N(3)-C(7)	115.6(3)	N(3)-C(10)-H(10)	119.0

Symmetry transformations used to generate equivalent atoms: #1 x+1,y,z #2 x-1,y,z

Table S2. Bond lengths (Å) and angles (°) for compound 2.

Bond distances	**atom-atom**	**distance**	**atom-atom**	**distance**	**atom-atom**	**distance**
	Hg(1)-N(4)	2.429(3)	C(5)-H(5)	0.9500	N(3)-C(4)	1.339(6)
	Hg(1)-Br(1)	2.4917(5)	C(6)-C(11)	1.395(6)	N(4)-C(7)	1.343(5)
	Br(1)-Hg(1)#2	3.0561(5)	C(9)-C(10)	1.378(6)	C(1)-C(2)	1.507(6)
	N(1)-C(1)	1.355(5)	C(10)-C(11)	1.383(6)	C(3)-H(3)	0.9500
	N(1)-H(1N)	0.80(5)	C(11)-H(11)	0.9500	C(4)-H(4)	0.9500
	N(2)-C(2)	1.344(5)	Hg(1)-Br(2)	2.4884(4)	C(6)-C(7)	1.392(6)
	N(3)-C(3)	1.341(5)	Hg(1)-Br(1)#1	3.0561(5)	C(7)-H(7)	0.9500
	N(4)-C(9)	1.350(5)	O(1)-C(1)	1.228(5)	C(9)-H(9)	0.9500
	C(2)-C(3)	1.380(6)	N(1)-C(6)	1.415(5)	C(10)-H(10)	0.9500
	C(4)-C(5)	1.384(6)	N(2)-C(5)	1.338(5)		
Bond angles	**atom-atom-atom**	**angle**	**atom-atom-atom**		**atom-atom-atom**	**angle**
	N(4)-Hg(1)-Br(2)	97.39(8)	C(7)-C(6)-C(11)	118.5(4)	O(1)-C(1)-N(1)	124.6(4)
	Br(2)-Hg(1)-Br(1)	164.073(16)	C(11)-C(6)-N(1)	123.0(4)	N(1)-C(1)-C(2)	116.1(4)
	Br(2)-Hg(1)-Br(1)#1	92.207(15)	N(4)-C(7)-H(7)	118.8	N(2)-C(2)-C(1)	118.9(4)
	Hg(1)-Br(1)-Hg(1)#2	88.889(15)	N(4)-C(9)-C(10)	121.9(4)	N(3)-C(3)-C(2)	122.5(4)
	C(1)-N(1)-H(1N)	118(4)	C(10)-C(9)-H(9)	119.0	C(2)-C(3)-H(3)	118.8
	C(5)-N(2)-C(2)	115.0(4)	C(9)-C(10)-H(10)	120.1	N(3)-C(4)-H(4)	118.9
	C(7)-N(4)-C(9)	118.6(4)	C(10)-C(11)-C(6)	118.6(4)	N(2)-C(5)-C(4)	122.6(4)
	C(9)-N(4)-Hg(1)	119.2(3)	C(6)-C(11)-H(11)	120.7	C(4)-C(5)-H(5)	118.7
	O(1)-C(1)-C(2)	119.3(4)	N(4)-Hg(1)-Br(1)	98.49(8)	C(7)-C(6)-N(1)	118.4(4)
	N(2)-C(2)-C(3)	122.4(4)	N(4)-Hg(1)-Br(1)#1	90.38(9)	N(4)-C(7)-C(6)	122.4(4)
	C(3)-C(2)-C(1)	118.7(4)	Br(1)-Hg(1)-Br(1)#1	88.889(15)	C(6)-C(7)-H(7)	118.8
	N(3)-C(3)-H(3)	118.8	C(1)-N(1)-C(6)	124.7(4)	N(4)-C(9)-H(9)	119.0
	N(3)-C(4)-C(5)	122.3(4)	C(6)-N(1)-H(1N)	118(4)	C(9)-C(10)-C(11)	119.9(4)
	C(5)-C(4)-H(4)	118.9	C(4)-N(3)-C(3)	115.2(4)	C(11)-C(10)-H(10)	120.1
	N(2)-C(5)-H(5)	118.7	C(7)-N(4)-Hg(1)	122.2(3)	C(10)-C(11)-H(11)	120.7

Symmetry transformations used to generate equivalent atoms: #1 x+1,y,z #2 x-1,y,z

Table S3. Bond lengths (Å) and angles (°) for compound 3.

Bond distances	**atom-atom**	**distance**	**atom-atom**	**distance**	**atom-atom**	**distance**
	Hg(1)-N(1)	2.585(13)	C(6)-C(10)	1.36(2)	N(2)-C(4)	1.30(2)
	Hg(1)-I(1)	2.6483(12)	N(3)-C(6)	1.449(19)	C(9)-H(9)	0.9292(0)
	Hg(1)-I (2)	2.6394(12)	N(3)-C(5)	1.38(2)	C(8)-H(8)	0.9298(0)
	N(4)-Hg(1)#1	2.458(14)	O(1)-C(5)	1.134(18)	C(7)-H(7)	0.9301(0)
	Hg(1)-N(4) #2	2.458(14)	C(5)-C(4)	1.54(2)	C(10)-H(10)	0.9309(0)
	N(4)-C(9)	1.29(2)	C(4)-C(1)	1.42(2)	N(3)-H(3A)	0.8596(0)
	N(4)-C(10)	1.35(2)	C(1)- N(1)	1.36(2)	C(1)-H(1)	0.9297(0)
	C(9)-C(8)	1.38(3)	C(2)- N(1)	1.33(2)	C(2)-H(2)	0.9304(1)
	C(8)-C(7)	1.40(2)	C(2)-C(3)	1.36(2)	C(3)-H(3)	0.9294(0)
	C(6)-C(7)	1.39(2)	C(3)- N(2)	1.37(2)		
Bond angles	**atom-atom-atom**	**angle**	**atom-atom-atom**		**atom-atom-atom**	**angle**
	N(4)-Hg(1)-I(1)#2	98.0(3)	O(1)- C(5)- N(3)	129.7(14)	C(2)-N(1)-Hg(1)	119.(1)
	I(2)-Hg(1)-I(1)	151.70(4)	N(1)-C(1)-C(4)	118.2(15)	N(2)-C(4)-C(1)	123.9(14)
	N(4)-Hg(1)-N(1) #2	109.4(4)	N(4)-C(9)-C(8)	121.7(16)	N(1)-C(2)-C(3)	121.7(15)
	N(4)-Hg(1)-I(2)#2	101.0(3)	O(1)-C(5)-C(4)	121.8(14)	C(9)-N(4)-C(10)	120.1(15)
	N(1)- Hg(1)- I(2)	97.0(3)	N(3)-C(5)-C(4)	108.4(12)	C(6)-C(7)-C(8)	115.2(16)
	N(1)-Hg(1)-I(1)	96.2(3)	N(4)-C(10)-C(6)	121.4(16)	C(9)-C(8)-C(7)	120.9(16)
	C(5)-N(3)-C(6)	123.7(13)	C(2)-C(3)-N(2)	121.7(15)	C(1)-C(4)-C(5)	117.6(15)
	C(1)-N(1)-Hg(1)	122.3(11)	C(2)-N(1)-C(1)	118.0(14)	N(2)-C(4)-C(5)	118.4(13)
	C(9)-N(4)-Hg(1)#1	120.2(11)	C(7)-C(6)-N(3)	123.9(15)	C(4)-N(2)-C(3)	115.7(13)
	C(10)-N(4)-Hg(1)#1	119.6(11)	C(10)-C(6)-N(3)	115.5(15)	C(10)-C(6)-C(7)	120.6(15)

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

Table S4. Bond lengths (Å) and angles (°) for compound 4.

Bond distances	**atom-atom**	**distance**	**atom-atom**	**distance**	**atom-atom**	**distance**
	Zn(1)-N(5)	2.0436(13)	C(9)-H(9)	0.9500	N(6)-H(6N)	0.852(19)
	Zn(1)-Cl(2)	2.2206(5)	C(11)-C(12)	1.393(2)	N(7)-C(18)	1.340(2)
	O(1)-C(6)	1.2229(19)	C(12)-C(13)	1.396(2)	N(8)-C(17)	1.336(2)
	N(1)-C(5)	1.340(2)	C(13)-H(13)	0.9500	C(1)-H(1)	0.9500
	N(2)-C(6)	1.355(2)	C(14)-H(14)	0.9500	C(3)-C(4)	1.377(2)
	N(2)-H(2N)	0.80(2)	C(16)-C(17)	1.501(2)	C(4)-C(5)	1.386(2)
	N(3)-C(8)	1.337(2)	C(18)-H(18)	0.9500	C(5)-H(5)	0.9500
	N(4)-C(7)	1.338(2)	C(19)-H(19)	0.9500	C(7)-C(8)	1.386(2)
	N(5)-C(11)	1.3468(19)	Zn(1)-N(1)	2.0497(12)	C(9)-C(10)	1.383(2)
	N(6)-C(12)	1.4029(19)	Zn(1)-Cl(1)	2.2309(4)	C(10)-H(10)	0.9500
	N(7)-C(19)	1.331(2)	O(2)-C(16)	1.2219(19)	C(11)-H(11)	0.9500
	N(8)-C(20)	1.335(2)	N(1)-C(1)	1.3458(19)	C(13)-C(14)	1.383(2)
	C(1)-C(2)	1.392(2)	N(2)-C(2)	1.407(2)	C(14)-C(15)	1.382(2)
	C(2)-C(3)	1.394(2)	N(3)-C(9)	1.335(2)	C(15)-H(15)	0.9500
	C(3)-H(3)	0.9500	N(4)-C(10)	1.335(2)	C(17)-C(18)	1.385(2)
	C(4)-H(4)	0.9500	N(5)-C(15)	1.342(2)	C(19)-C(20)	1.382(2)
	C(6)-C(7)	1.502(2)	N(6)-C(16)	1.360(2)	C(20)-H(20)	0.9500
	C(8)-H(8)	0.9500				
Bond angles	**atom-atom-atom**	**angle**	**atom-atom-atom**	**angle**	**atom-atom-atom**	**angle**
	N(5)-Zn(1)-N(1)	103.66(5)	C(11)-C(12)-N(6)	122.73(14)	C(4)-C(3)-H(3)	120.5
	N(1)-Zn(1)-Cl(2)	109.18(4)	C(14)-C(13)-C(12)	119.29(14)	C(3)-C(4)-C(5)	119.59(15)
	N(1)-Zn(1)-Cl(1)	106.93(4)	C(12)-C(13)-H(13)	120.4	C(5)-C(4)-H(4)	120.2
	C(5)-N(1)-C(1)	119.37(13)	C(15)-C(14)-H(14)	120.5	N(1)-C(5)-H(5)	119.2
	C(1)-N(1)-Zn(1)	122.64(10)	N(5)-C(15)-C(14)	122.06(14)	O(1)-C(6)-N(2)	125.09(15)
	C(6)-N(2)-H(2N)	115.1(14)	C(14)-C(15)-H(15)	119.0	N(2)-C(6)-C(7)	113.37(13)
	C(9)-N(3)-C(8)	115.86(16)	O(2)-C(16)-C(17)	121.35(14)	N(4)-C(7)-C(6)	117.28(14)
	C(15)-N(5)-C(11)	119.53(13)	N(8)-C(17)-C(18)	122.41(14)	N(3)-C(8)-C(7)	121.46(16)
	C(11)-N(5)-Zn(1)	120.34(10)	C(18)-C(17)-C(16)	119.40(13)	C(7)-C(8)-H(8)	119.3
	C(16)-N(6)-H(6N)	116.5(13)	N(7)-C(18)-H(18)	119.1	N(3)-C(9)-H(9)	118.5
	C(19)-N(7)-C(18)	115.73(14)	N(7)-C(19)-C(20)	122.47(15)	N(4)-C(10)-C(9)	120.93(15)
	N(1)-C(1)-C(2)	121.72(14)	C(20)-C(19)-H(19)	118.8	C(9)-C(10)-H(10)	119.5
	C(2)-C(1)-H(1)	119.1	N(8)-C(20)-H(20)	119.0	N(5)-C(11)-H(11)	119.2
	C(1)-C(2)-N(2)	123.06(14)	N(5)-Zn(1)-Cl(2)	106.99(4)	C(11)-C(12)-C(13)	118.57(14)

C(4)-C(3)-C(2)	118.90(14)	N(5)-Zn(1)-Cl(1)	111.97(4)	C(13)-C(12)-N(6)	118.67(13)
C(2)-C(3)-H(3)	120.5	Cl(2)-Zn(1)-Cl(1)	117.259(17)	C(14)-C(13)-H(13)	120.4
C(3)-C(4)-H(4)	120.2	C(5)-N(1)-Zn(1)	117.94(10)	C(15)-C(14)-C(13)	119.03(14)
N(1)-C(5)-C(4)	121.67(14)	C(6)-N(2)-C(2)	126.87(14)	C(13)-C(14)-H(14)	120.5
C(4)-C(5)-H(5)	119.2	C(2)-N(2)-H(2N)	118.0(14)	N(5)-C(15)-H(15)	119.0
O(1)-C(6)-C(7)	121.51(14)	C(10)-N(4)-C(7)	116.51(14)	O(2)-C(16)-N(6)	124.91(14)
N(4)-C(7)-C(8)	122.17(15)	C(15)-N(5)-Zn(1)	119.91(10)	N(6)-C(16)-C(17)	113.70(13)
C(8)-C(7)-C(6)	120.52(14)	C(16)-N(6)-C(12)	126.31(13)	N(8)-C(17)-C(16)	118.17(13)
N(3)-C(8)-H(8)	119.3	C(12)-N(6)-H(6N)	117.1(13)	N(7)-C(18)-C(17)	121.72(14)
N(3)-C(9)-C(10)	123.03(16)	C(20)-N(8)-C(17)	115.59(14)	C(17)-C(18)-H(18)	119.1
C(10)-C(9)-H(9)	118.5	N(1)-C(1)-H(1)	119.1	N(7)-C(19)-H(19)	118.8
N(4)-C(10)-H(10)	119.5	C(1)-C(2)-C(3)	118.67(14)	N(8)-C(20)-C(19)	122.06(15)
N(5)-C(11)-C(12)	121.51(14)	C(3)-C(2)-N(2)	118.27(14)	C(19)-C(20)-H(20)	119.0
C(12)-C(11)-H(11)	119.2				

Table S5. Bond lengths (Å) and angles (°) for compound 5.

Bond distances	**atom-atom**	**distance**	**atom-atom**	**distance**	**atom-atom**	**distance**
	N(1) -Cd(1)	2.375(7)	C(2) -C(1)	1.398(12)	C(5)-C(4)	1.385(12)
	Cd(1)-N(1) #1	2.375(7)	C(2)-C(3)	1.393(12)	N(3)-C(8) #4	1.341(14)
	Cd(1)-I(1) #2	2.962(1)	C(4) -C(3)	1.394(11)	C(9) -N(3)	1.340(14)
	Cd(1)-I(1) #3	2.962(1)	N(2)-C(6)	1.360(12)	N(4)-C(10) #5	1.343(13)
	Cd(1)-I(1) #1	2.9715(10)	C(6)-O(1)	1.226(13)	C(8)-N(3) #5	1.341(14)
	Cd(1)-I(1)	2.9716(10)	C(6)-C(7)	1.505(12)	C(10)-N(4) #4	1.343(13)
	I(1)-Cd(1)	2.9621(10)	C(2)-N(2)	1.409(11)	C(9)-C(10)	1.372(15)
	C(7)-N(4)	1.333(13)	N(1)-C(5)	1.345(11)		
	C(7)-C(8)	1.394(14)	N(1)-C(1)	1.345(10)		
Bond angles	**atom-atom-atom**	**angle**	**atom-atom-atom**	**angle**	**atom-atom-atom**	**angle**
	N(1)-Cd(1)-N(1)#1	179.6(6)	C(5)- N(1) -C(1)	119.2(7)	C(2)-C(3)-C(4)	118.8(8)
	N(1)-Cd(1)-I(1) #1#2	90.7(2)	C(5)-N(1)-Cd(1)	119.5(5)	O(1)-C(6)-N(2)	124.4(9)
	N(1)-Cd(1)-I(1) #2	89.6(2)	C(1)-N(1)-Cd(1)	121.3(6)	O(1)-C(6)-C(7)	120.0(9)
	N(1)-Cd(1)-I(1) #1#3	89.6(2)	C(3)-C(2)-C(1)	119.2(8)	N(2)-C(6)-C(7)	115.5(9)
	N(1)-Cd(1)-I(1) #3	90.7(2)	N(1)-C(5)-C(4)	122.5(8)	N(4)-C(7)-C(8)	123.0(9)
	C(6)-N(2)-C(2)	124.7(8)	C(3)-C(2)-N(2)	119.2(8)	N(4)-C(7)-C(6)	119.5(9)
	I(1)-Cd(1)-I(1) #2#3	94.39(4)	C(5)-C(4)-C(3)	118.8(8)		
	N(1)-Cd(1)-I(1) #1#1	89.3(2)	C(7)-N(4)-C(10)#5	115.0(9)		
	N(1)-Cd(1)-I(1) #1	90.4(2)	C(1)-C(2)-N(2)	121.6(8)		
	I(1)-Cd(1)-I(1) #2#1	179.80(4)	N(1)-C(1)-C(2)	121.4(8)		
	I(1)-Cd(1)-I(1) #3#1	85.804(16)	N(3)-C(9)-C(10)	122.5(9)		
	N(1)-Cd(1)-I(1) #1	90.4(2)	C(9)- N(3) -C(8)#4	115.8(9)		
	N(1)-Cd(1)-I(1)	89.3(2)	N(3)-C(8)-C(7) #5	121.1(10)		
	I(1)-Cd(1)-I(1) #2	85.801(16)	N(4)-C(10)-C(9)#4	122.5(10)		
	C(8)-C(7)-C(6)	117.5(9)				
	I(1)-Cd(1)-I(1) #3	179.80(4)				
	I(1)-Cd(1)-I(1) #1	94.00(4)				
	Cd(1)-I(1)-Cd(1) #6	85.799(16)				

Symmetry transformations used to generate equivalent atoms: #1 2-x, -y, z # 2 x, y, 1+z # 3 2-x, -y, 1+z #4 1/4+x, 1/4-y, 1/4+z #5 -1/4+x, 1/4-y, -1/4+z #6 x, y, -1+z

TableS6. π interaction parameters (Å and **°**) for compound 1-5

Compound	π...π	d_{Cg-Cg}	$d_{plane-plane}$	α	γ,β	d_{offset}
$[HgCl_2(L)]_n$(1)	$\pi_{py}...\pi_{py}$ [a]	3.8092(4)	3.5907	0.000(162)	19.50	1.27
	$\pi_{pz}...\pi_{pz}$ [a]	3.8092(4)	3.3300	0.000(129)	29.05	1.85
$[HgBr_2(L)]_n$(2)	$\pi_{py}...\pi_{py}$ [a]	3.9055(4)	3.6786	0.000(177)	19.62	1.31
	$\pi_{pz}...\pi_{pz}$ [a]	3.9055(4)	3.4177	0.000(176)	28.94	1.89
$[HgI_2(L)]_n$ (3)	halogen...π_{pz} [a]	3.9233(2)	3.6576	75.132(1)	68.79	1.42
	C5O1 ...π_{py}	3.5441(1)	3.534	4.30	-	0.27
$[ZnCl_2(L)]_n$ (5)	$\pi_{py}...\pi_{py}$ [b]	3.7474(3)	3.7162	0.000(175)	7.40	0.48
	$\pi_{py}...\pi_{py}$ [c]	3.4374(2)	3.4032	0.000(81)	8.09	0.48
	C6O1 ...π_{pz} [d]	3.8853(3)	3.7867	12.93	-	0.87
	C16O2...π_{pz} [e]	3.8293(3)	3.6118	19.40	-	1.27
$[CdI_2(L)]_n$ (4)	$\pi_{py}...\pi_{py}$ [f]	4.0392(5)	4.0207	0.000	5.48	0.38
	$\pi_{pz}...\pi_{pz}$ [f]	4.0392(5)	3.5224	0.000(9)	29.30	1.97

Symmetry codes: [a] -1+x, y, z. [b] -x, 1-y, 2-z. [c] -x, 1-y, 1-z. [d] 1-x, -y, 2-z. [e] 1-x, -y, 1-z. [f] x, y, -1+z.

Table S7. Angles between Py, Pz and Amide planes in compounds 1-5.

Table S8. Mercury (II) halide (halide= Cl(1-37), Br(38-76), and I(77-100)) coordination compounds containing pyrazine-type organic ligand.

NO.	Refcode	N_{Pz}-coord.	Pyridine containe	N_{Py}-coord.	coordination geometry of Hg	Hg-Npz distance	Hg-Npy distance	Hg-$X_{terminal}$ (X= Cl,Br,I)	Hg-$X_{bridging}$ (X= Cl,Br,I)	Ref.
	Compound			**< Py and Amide plane (°)**		**<Pz and Amide plane(°)**		**<Py and Pz (°)**		
1	EREQEZ	× pz	✓	✓	fourfold coordination	-	2.590 (5)	2.3464 (16)	-	**1**
	$[HgCl_2(L)]_n$(1)			29.38	geometry square-planar	3.74	2.876 (5)	32.59		
2	BABLOH	✓pz	✓py	✓	Three-coord.	2.633(8)	2.527(7)	2.315(3)	2.357(2)	**2**
	$[HgBr_2(L)]_n$(2)			29.89	square pyramid	4.30		2.361(2)	2.359(2)	
					octahedral					
	$[HgI_2(L)]_n$ (3)			7.24		7.06		14.21		
3	BABLUN	✓pz	✓py	✓	octahedral	2.647	2.285	2.325(3)	3.149(2)	**2**
	$[ZnCl_2(L)_2]$ (4)			19.96(n1)		4.81(n3n4)		17.56(n1n3n4)	3.130(3)	
				19.47(n5)		8.21(n7n8)		25.58(n5n7n8)	2.362(2)	
									2.826(2)	
4	CEKHUX	✓pz	×	×	octahedral	2.812(5)	-	2.304(2)	-	**3**
5	CEKJOT	**$[CdI_2(L)_2]n$ (5)**	×	×	28.07	square-based pyramidal	1.98	2.315(2)	26.79	-	**3**
					square-planar	2.760(6)		2.316(2)		
					square-planar	2.723(6)		2.319(2)		
						2.713(5)		2.312(2)		
6	CIDLOS	✓pz	×	×	octahedral	2.644(6)	-	-	2.382(2)	**4**
									3.099(2)	
7	CIDMEJ	✓pz	×	×	square pyramid	2.616(9)	-	2.316(4)	2.336(4)	**4**
8	CIDMUZ	✓pz	×	×	distorted octahedral	2.657(4)	-	-	2.368(1)	**4**
									3.012(1)	
9	HIGQUL	✓pz	×	×	distorted octahedral	2.619(2)	-	-	2.377(1)	**4**
									2.983(1)	
10	CUYDUW	✓pz	×	×	octahedral	2.844(4)	-	2.2931(11)	-	**5**
11	DEBVAJ	×Pz(s)	×	×	Five-coordinate	-	-	2,3068(11)	-	**6**
								2,3107(11)		
12	DEBWEN	-	×	×	Six-coordinate	-	-	2,3396(10)	-	**6**
		Pz(s)						2,3396(11)		
13	EJOPEZ	✓	×	×	trigonal bipyramidal	2.507(7)	-	2.2901(2)	2.3274(1)	**7**
		pz			trigonal bipyramidal	2.7294(1)			3.0603(1)	
						2.568(7)				
						2.7873(1)				

14	EMIGAK	✓ pz	×	×	Seesaw	2.532(6)	-	2.298(2) 2.309(2)	-	**8**
15	EMIPAT	✓ pz	×	×	Seesaw	2.522(6)	-	2.299(2) 2.297(2)	-	**8**
16	EWIPIK	✓ pz	✓py	✓	distorted square pyramid	2.783(10) 2.701(11)	2.483(9)	2.343(3) 2.323(3)	-	**9**
17	EWOQUC	✓ pz	×	×	octahedral	2.510 (7)	-	-	2.503 (3) 2.842 (4)	**10**
18	FECHEC	×pz	✓py	×	tetrahedral	-	-	2.476(2)	-	**11**
19	GAVBOV	✓pz	✓py	✓	five-coordinated	2.610 (4)	2.539 (4) 2.622 (4)	2.3569 (14) 2.3773 (14)	-	**12**
20	GURKOU	✓pz	×	×	Four -coordinate linear geometry	2.788(4)	-	2.2975(10)	-	**13**
21	HOTBID	✓pz	✓ QUINOLIN	✓	highly distorted trigonal bipyramid	2.631(6) 2.647(6)	2.380(6) 2.393(5)	2.364(2) 2.348(2) 2.348(2) 2.354(2)	-	**14**
22	IQIHUM	✓pz	×	×	highly distorted tetrahedral	2.463(6) 2.491(5)	-	2.324(2) 2.342(2)	-	**15**
23	KABRUC	✓pz	×	×	trigonal bipyramidal distorted octahedral	2.773(3)	-	2.330(1)	-	**16**
24	QEZNIU	✓pz	×	×	seesaw	2.656(8)	-	2.289(2) 2.303(2)	-	**17**
25	QEZNOA	✓pz	×	×	square-based pyramid	2.575(5)	-	-	2.3464(18) 3.047(2) 2.3375(19) 3.044(2)	**17**
26	QEZNUG	✓pz	×	×	three coordination seesaw	2.573(2) 2.516(2)	-	2.3106(6) 2.3089(7) 2.3340(7) 2.3088(7)	-	**17**
27	QEZPAO	✓pz	×	×	three coordination seesaw	2.599(7) 2.551(9)	-	2.294(2) 2.295(2) 2.300(2) 2.325(2)	-	**17**
28	QIVXAV	✓Quinoxaline	✓py	✓	Four-coordinate Four-coordinate	2.651 2.831	2.445 2.491	2.317(3) 2.329(2)	2.366(2) 2.367(2)	**18**
29	QUMVIE	✓Pz(s)	×	×	Five- coordinate	2.561(13)	-	-	2.348(4) 2.343(4) 3.08(4) 2.994(5)	**19**
30	QUVXEM	✓ phenazine	×	×	distorted square pyramidal	2.595(7)	-	-	2.334(1) 2.338(2) 3.059(2) 3.104(2)	**20**
31	RUSNEZ	✓Pz	×	×	Distorted octahedral	2.661 (7)	-	-	2.970 (2) 2.375 (2)	**21**
32	SAXDOK	✓2-Methylquinoxaline	×	×	Distorted octahedral	2.61(3)	-	-	2.348(7) 2.326(7) 3.081(7) 3.070(7) 3.328(7)	**22**
33	TIZNIB	✓pz	×	×	seesaw	2.657(7)	-	2.298(2) 2.301(2)	-	**23**
34	XIVKIW	✓ pz	×	×	three-coordinate	2.548(9)	-	2.302(3) 2.318(3)	-	**24**
35	XIVKOS	✓pz	×	×	three-coordinate	2.556(8)	-	2.305(3) 2.313(3)	-	**24**
36	YIZTUW	✓quinoxaline,	✓py	✓	distorted square pyramidal	2.480(4)	2.336(10)	2.387(4)	2.500(4) 2.742(3)	**25**
37	ZUFHUF	✓benzo[*a*]quinoxalino[2,3-*c*]phenazine	×	×	distorted tetrahedral	2.572(5)	-	2.3624(16)	-	**26**
38	IVOKIP	✓ polyphenyl quinoxaline	×	×	deformed tetrahedral	2.585(4) 2.606(4)	×	2.4519(9) 2.4531(10)	×	**27**
39	BUKYEN	✓	×	×	three-coordinate ,T-shaped	2.526(12)	×	2.4516(14)	×	**28**

		pz						2.4309(14)		
40	BUKYIR	✓ pz	×	×	three-coordinate , T-shaped	2.552(14)	×	2.4208(18) 2.4507(16)	×	**28**
41	CEKJAF	✓ pz	×	×	square-based pyramid	2.447(1)	×	2.455(1)	2.472(2) 3.112(1)	**3**
42	CEKJIN	✓ pz	×	×	three-coordinate	2.538(7)	×	2.413(1) 2.445(1)	×	**3**
43	CIDLUY	✓ pz	×	×	distorted square pyramidal	2.445(16)	×	×	2.475(4) 2.474(4) 3.148(3) 3.191(3)	**4**
44	CIDMIN	✓ pz	×	×	distorted octahedral	2.734(6)	×	×	2.459(2) 3.280(2)	**4**
45	CIDNAG	✓ pz	×	×	seesaw	×	×	2.418(1) 2.427(1)	×	**4**
46	CIDNEK	✓ pz	×	×	distorted octahedral	2.695(1)	×	×	2.483(1) 3.181(1)	**4**
47	COTSAH	✓ phenazine	×	×	distorted tetrahedral	2.477(4) 2.534(4)	×	2.4534(12) 2.4595(15)	×	**29**
48	CUMXIT	✓ quinoxaline	✓ PY	✓	distorted tetrahedral	2.542(7)	2.471(8)	2.4661(12) 2.4702(13)	×	**30**
49	CUYFEI	✓ pz	×	×	Four-coordinate	2.584(6)	×	2.4244(11) 2.4260(13)	×	**5**
50	DULWAJ	✓ pz	×	×			×	×		**31**
51	EMIFUD	✓ pz	×	×	seesaw geometry	2.528(6)	×	2.422(1) 2.425(1)	×	**8**
52	EMINUL	✓ pz	×	×	T-shape geometry	2.494(2)	×	2.413(3) 2.450(3)	×	**8**
53	EWIPEG	✓ pz	✓ PY	✓	Distorted tetrahedral	2.496(9)	2.419(11)	2.4713(14) 2.465(13)	×	**9**
54	EWORAJ	✓ pz	×	×	Deformed octahedral	2.719 (4) 2.844 (4)	×	2.4691 (10) 2.4726 (9)	×	**32**
55	GURKUA	✓ quinoxaline	×	×	linear geometry	2.802(3)	×	2.4203(4)	×	**13**
56	HOTBUP	✓ pz	✓ quinolin	✓	distorted octahedron trigonal pyramidal	2.756(1)	2.366(7)	2.4247(9) 2.4597(13)	2.5181(11) 3.0667 (12)	**14**
57	HOTCAW	✓ pz	✓ quinolin	×	distorted octahedron	2.720(9)	×	×	2.4870(12) 3.1150(13)	**14**
58	IQIJAU	✓ pz	×	×	distorted tetrahedral	2.499(1) 2.571(1)	×	2.266(1) 2.332(1)	×	**15**
59	MIRPUZ	✓ pz	×	×	distorted tetrahedral	2.528 (13)	×	2.4234 (15)	×	**33**
60	MOWGEL	✓ bpyz	×	×	distorted octahedron	2.723	×	×	2.4683(7) 3.194	**34**
61	OMILED	× phenazine	×	×	tetrahedral	×	×	2.571(2) 2.624(2)	×	**35**
62	OROJIP	× quinoxaline	×	×	Distorted tetrahedral	×	×	2.5527(14) 2.5175(14)	×	**36**
63	QEZPES	✓ pz	×	×	seesaw geometry	2.514(7)	×	2.4147(10) 2.4293(0)	×	**17**
64	QEZPIW	✓ pz	×	×	T-shaped	2.49(3)	×	2.443(4) 2.462(4)	×	**17**
65	QEZPOC	✓ pz	×	×	T-shaped	2.469(10)	×	2.4639(12) 2.4287(14)	×	**17**
66	QEZPUI	✓ pz	×	×	T-shaped	2.480(13)	×	2.424(2) 2.459(2)	×	**17**
67	QEZQAP	✓ pz	×	×	T-shaped	2.449(13)	×	2.420(2) 2.4569(18)	×	**17**
68	QIVWAU	× quinoxaline	✓ PY	✓	Four-coordinate	×	2.528(5)	2.488(1)	×	**18**
69	QUMTOI	✓ pz	×	×	distorted octahedral	2.476(10)	×	×	2.6668(14) 2.6669(14) 2.8748(14)	**19**
70	QUMTUO	✓ pz	×	×	distorted octahedron	2.568	×	×	2.4581(19) 2.4546(19) 3.132(2)	**19**

71	QUMVEA	✓ pz	×	×	distorted square pyramidal	2.508(13)	×	×	2.4800(16) 3.0700(16) 2.4783(16)	**19**
72	QUVWEL	✓ phenazine	×	×	square pyramidal	2.784(3)	×	×	2.4458(4) 2.4363(4) 3.1108(5) 3.3527(5)	**20**
73	QUVZUE	✓ phenazine	×	×	square pyramids	2.563(9)	×	×	2.461(1) 2.4634(9) 3.262(1) 3.296(1)	**20**
74	TIZNOH	✓ pz	×	×	seesaw	2.672(8)	×	2.426(1) 2.428(1)	×	**23**
75	ZATJOT	✓ quinoxaline	✓ PY	✓	distorted trigonal bipyramidal	2.489(16	2.366(16)	2.524(2	2.588(2 2.917(2	**37**
76	HULVOA	× quinoxaline	×	×	distorted tetrahedral	×	×	2.496(3)	2.776(4)	**38**
77	CEKHOR	✓ Pz	×	×	square-based pyramid	2.513(7)	×	2.611(1)	2.632(1) 3.501(1) 3.542(1)	**3**
78	CEKJET	✓ Pz	×	×	Distorted T-shape.	2.561(7)	×	2.586(1) 2.608(1)	×	**3**
79	CIDLIM	✓ Pz	×	×	distorted T-shape	2.662(9)	×	2.593(1) 2.594(1)	×	**4**
80	CIDMAF	✓ Pz	×	×	pseudo four-coordinate, seesaw geometry	2.659(5)	×	2.583(1) 2.599(1)	×	**4**
81	CIDMOF	✓ Pz	×	×	pseudo four-coordinate, seesaw geometry	2.628(5)	×	2.585(1) 2.593(1)	×	**4**
82	CUYFAE	✓ Pz	×	×	distorted octahedron	2.498(7)	×	2.6014(9) 2.6257(9)	×	**5**
83	EMIFOX	✓ Pz	×	×	T-shape	2.544(8)	×	2.596(1) 2.598(1)	×	**8**
84	EMINOF	✓ Pz	×	×	T-shape	2.537(2)	×	2.576(2) 2.604(2)	×	**8**
85	EWOREN	✓ Pz	×	×	Three-coordinate	2.511 (18)	×	2.6036 (19) 2.6278 (19)	×	**39**
86	EWOREN01	✓ Pz	×	×	distorted octahedron	2.507(10)	×	2.6121(9)	2.6388(8) 3.480	**19**
87	GAHPIR	✓ Pz	✓ PY	✓	Five-coordinate	2.635	2.547 2.583	2.631 2.669	×	**40**
88	HIGRAS	✓ Pz	×	×	distorted octahedral	2.887(2)	×	×	2.609(1) 3.544(1)	**4**
89	HOTBOJ	✓ Pz	✓ quinolin	✓	pseudo-six coordinate octahedral trigonal pyramidal	2.887(11)	2.391(9)	2.642(1) 2.5791(12)	2.7009(8) 3.1182(9)	**14**
90	HOTCEA	✓ Pz	✓ quinolin	×	T-shape	2.521(1)	×	2.599(1) 2.602(1)	×	**14**
91	IQIJEY	✓ Pz	×	×	Distorted tetrahedral	2.476	×	2.607(1)	2.614(1) 3.501(1)	**15**
92	IWEVIP	× Pz	✓ PY	✓	tetrahedral	×	2.443(4) 2.480(5)	2.6479(5) 2.6474(5)	×	**41(59)**
93	LAMVEC	✓ Pz	×	×	distorted tetrahedral	2.497 (11)	×	2.6373 (13)	×	**42**
94	QAMXIL	× Pz	×	×	Distorted tetrahedral	×	×	2.603(2) 2.633(2)	×	**43**
95	QEZQET	✓ Pz	×	×	seesaw	2.54(3)	×	2.602(2)	2.622(2) 3.512(3)d	**17**
96	QEZQIX	✓ Pz	×	×	square-based pyramid	2.474(10)	×	2.5950(11)	2.6381(10) 3.4957(5)	**17**
97	QEZQOD	✓ Pz	×	×	square-based pyramid	2.484(7)	×	25953(8)	2.6394(8) 3.5182(4)	**17**
98	QIVWIC	× quinoxaline	✓ PY	✓	tetrahedral	×	238,5(22) 244,3(22)	264,6(3) 264,9(3)	×	**18**
99	TIZNUN	✓ Pz	×	×	pseudo-square planar	2.94(1)	×	2.576(1)	×	**23**
100	ZOGWIB	✓ quinoxaline	✓ PY	✓	distorted square pyramid	2.541(18)	2.399(18)	2.671(2)	2.690(2) 3.416(1)	**44**

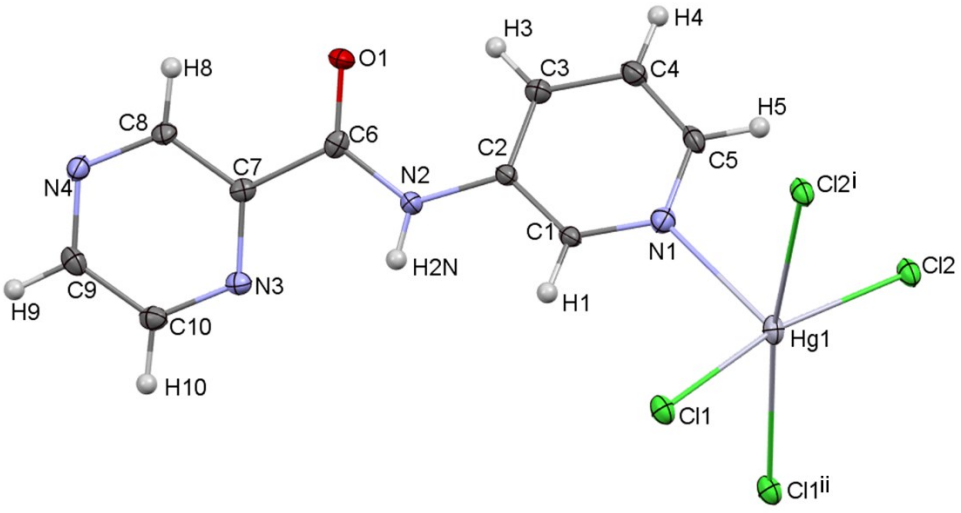

Figure S1. ORTEP diagram of compound **1**, showing coordination geometry. Ellipsoids are drawn at 50% probability level. Symmetry codes: i: 1+x, y, z, ii=-1+x, y, z.

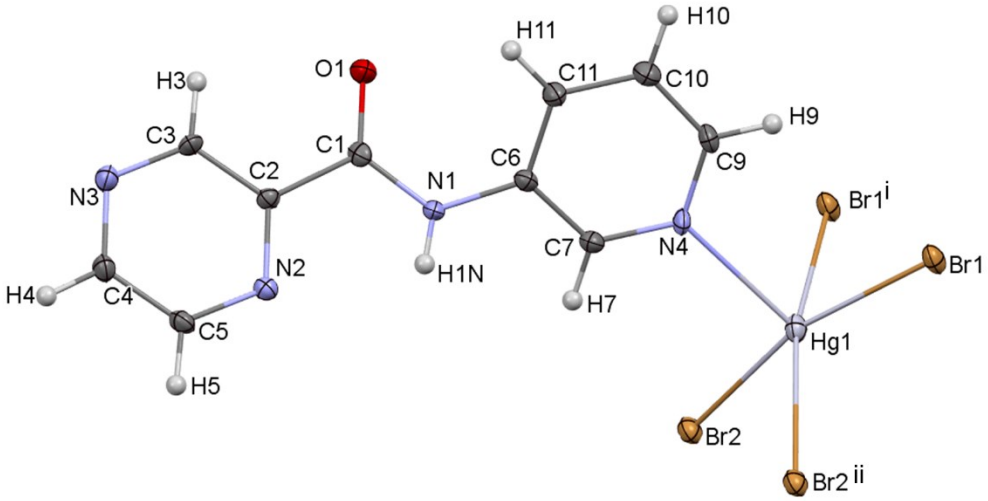

Figure S2. ORTEP diagram of compound **2**, showing coordination geometry. Ellipsoids are drawn at 50% probability level. Symmetry codes: i: 1+x, y, z, ii=-1+x, y, z.

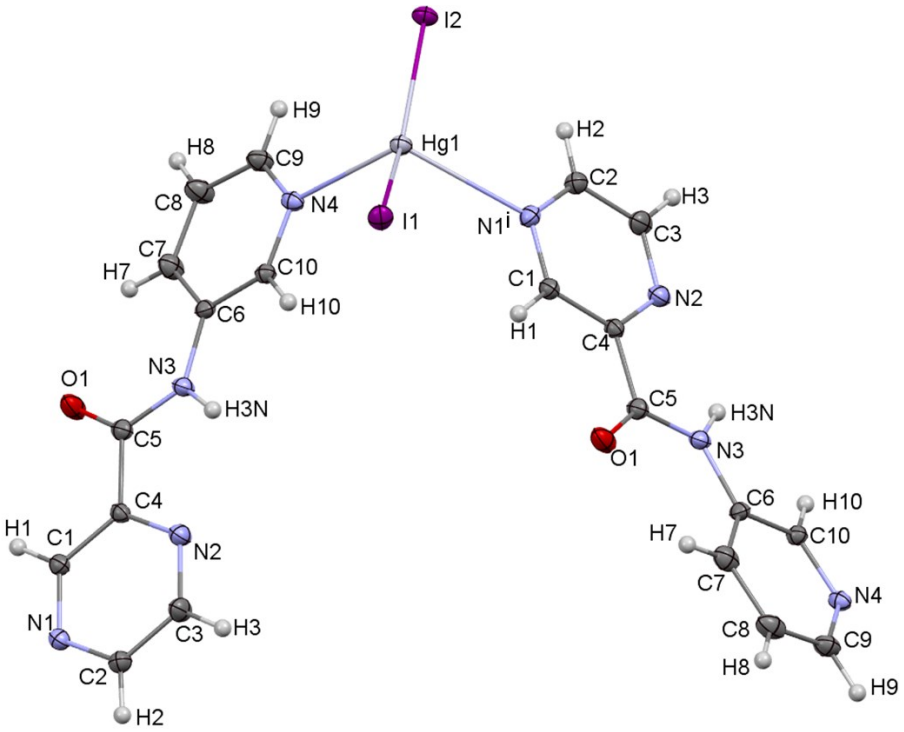

Figure S3. ORTEP diagram of compound **3**, showing coordination geometry. Ellipsoids are drawn at 50% probability level. Symmetry code: i= 2-x, -1/2+y, 1.5-z.

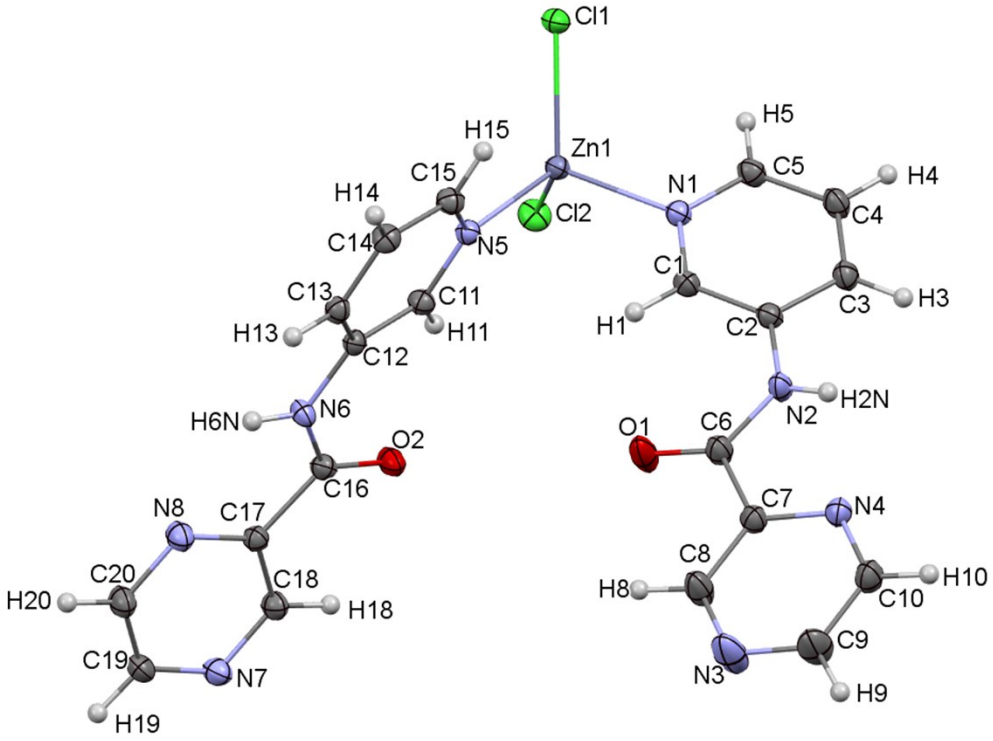

Figure S4. ORTEP diagram of compound **4**, showing coordination geometry. Ellipsoids are drawn at 50% probability level.

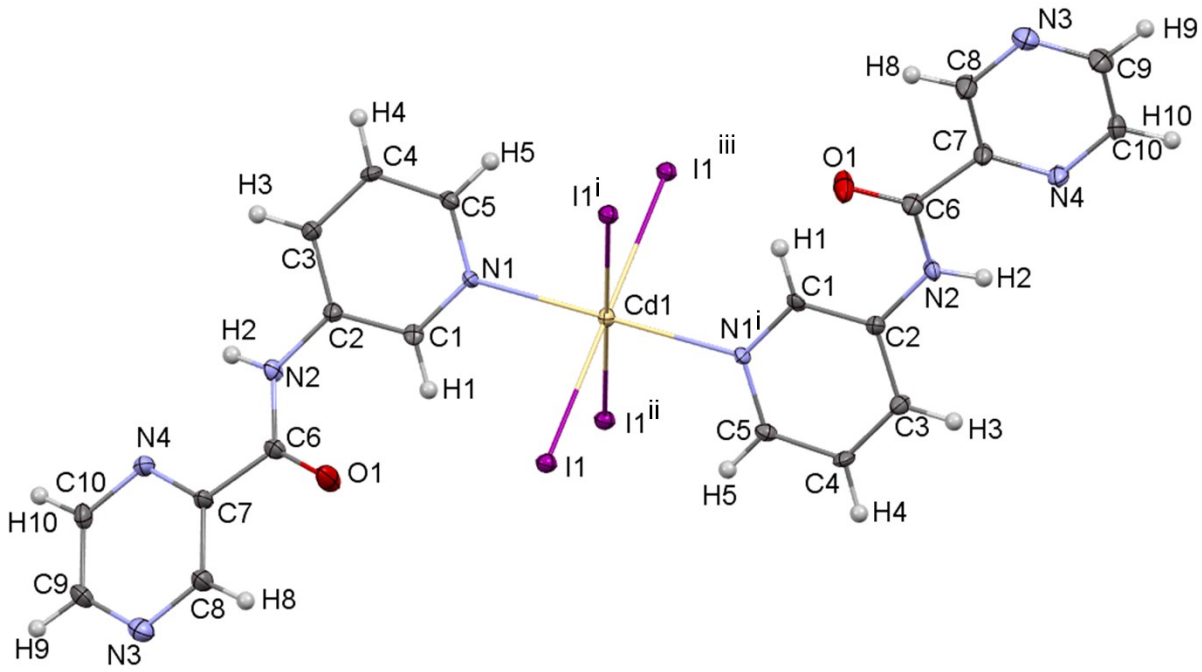

Figure S5. ORTEP diagram of compound **5**, showing coordination geometry. Thermal ellipsoids are drawn at 50% probability level. Symmetry codes: i: 2-x, -y, z, ii: x, y, 1+ z, iii: 2-x, -y, 1+z.

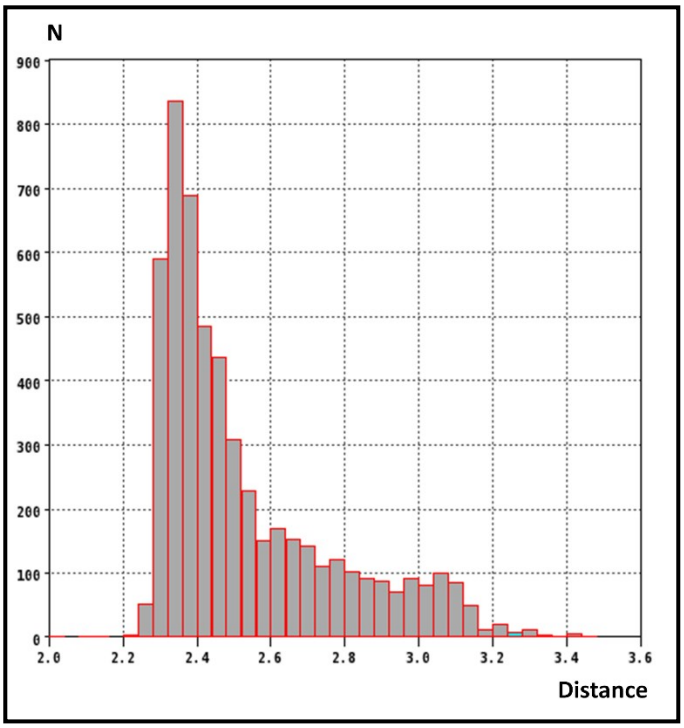

Figure S6. Histogram plot for Hg-Cl distance from a CSD search.

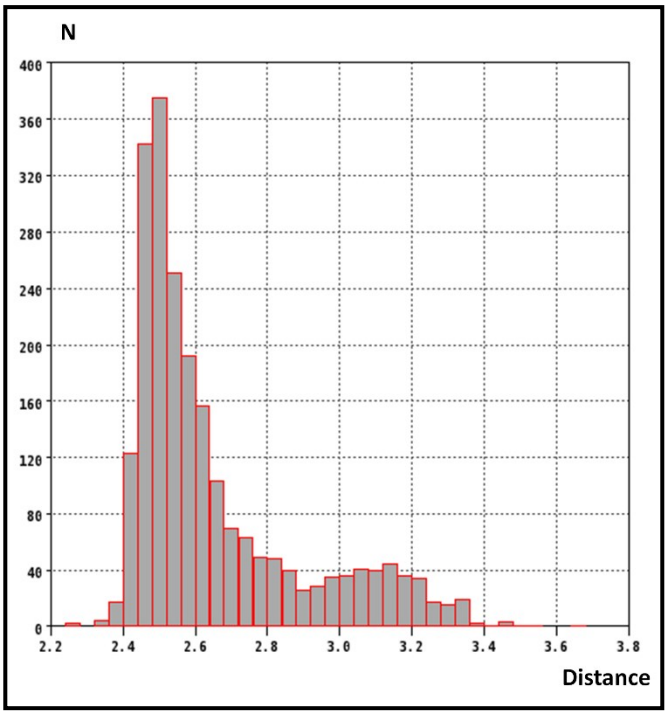

Figure S7. Histogram plot for Hg-Br distance from a CSD search.

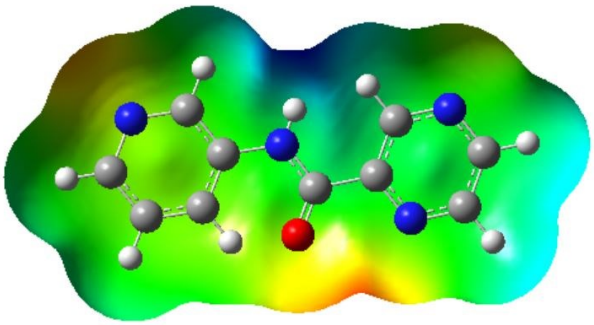

Figure S8. Electrostatic surface potentials (ESP) for ligand.

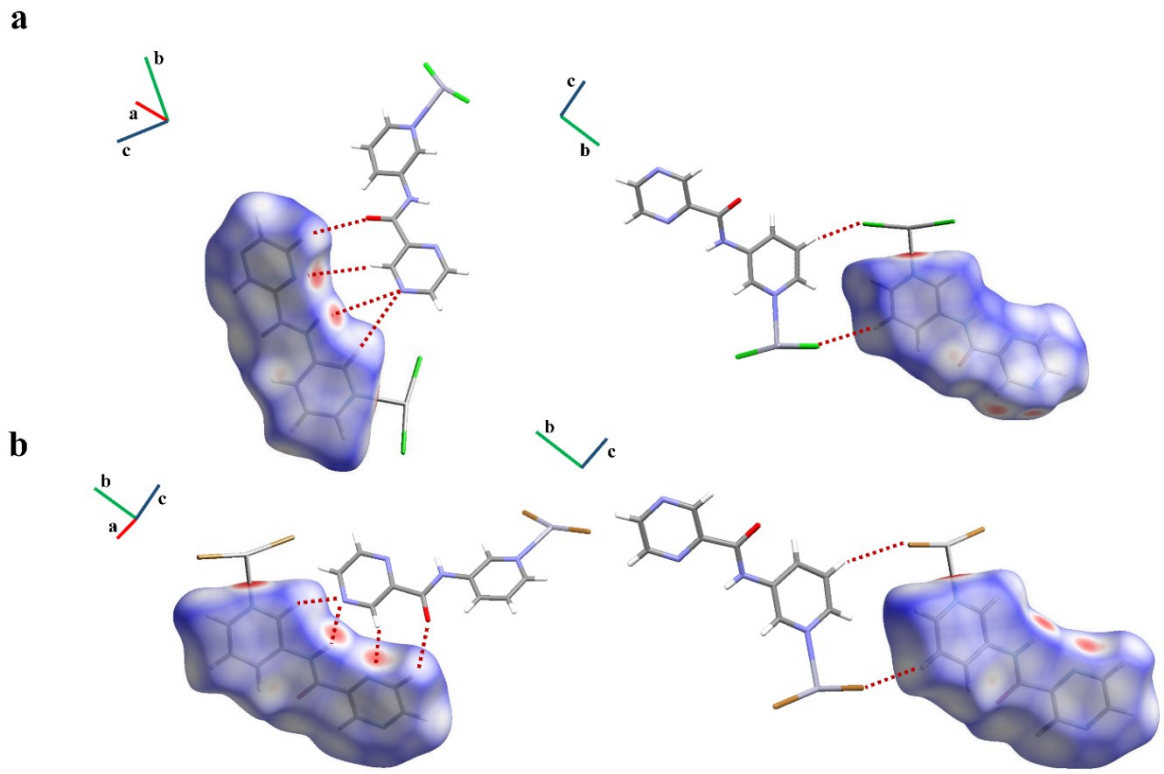

Figure S9. Hirshfeld surface mapped with d_{norm} for compound 1(top) and for compound 2 (bottom), showing C-H…O, C-H…N, N-H…N (left) and C-H…Cl (right) hydrogen bonds.

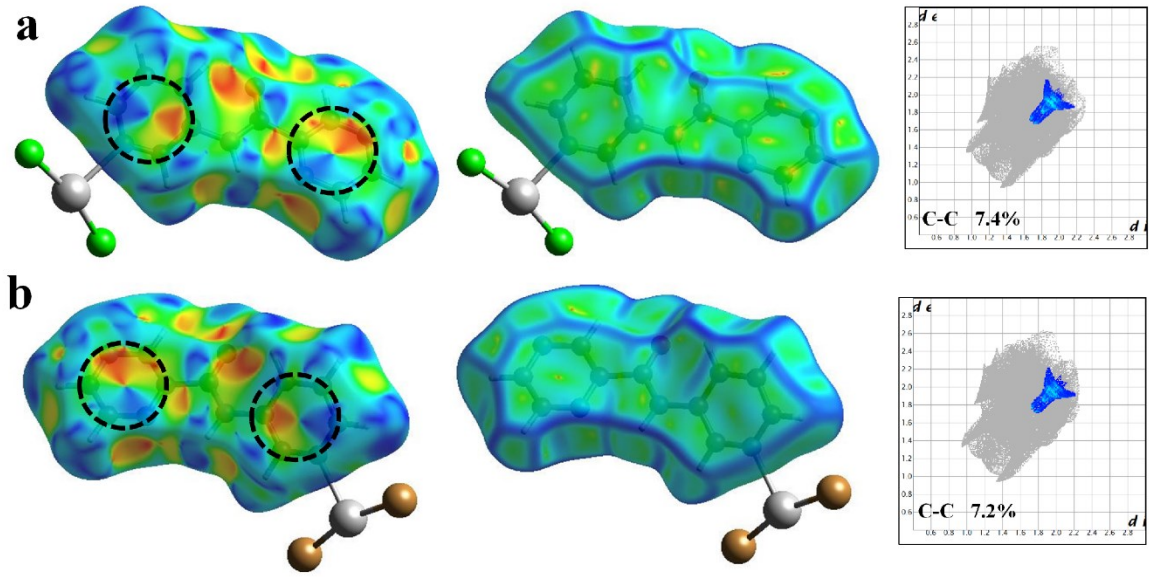

Figure S10. Hirshfeld surfaces mapped with shape index (red and blue triangles has been shown by black circle), curvedness and decomposed finger print plots to C-C contacts showing relative contribution of π•••π stacking interactions for compound **1**(a), **2**(b), (left to right)

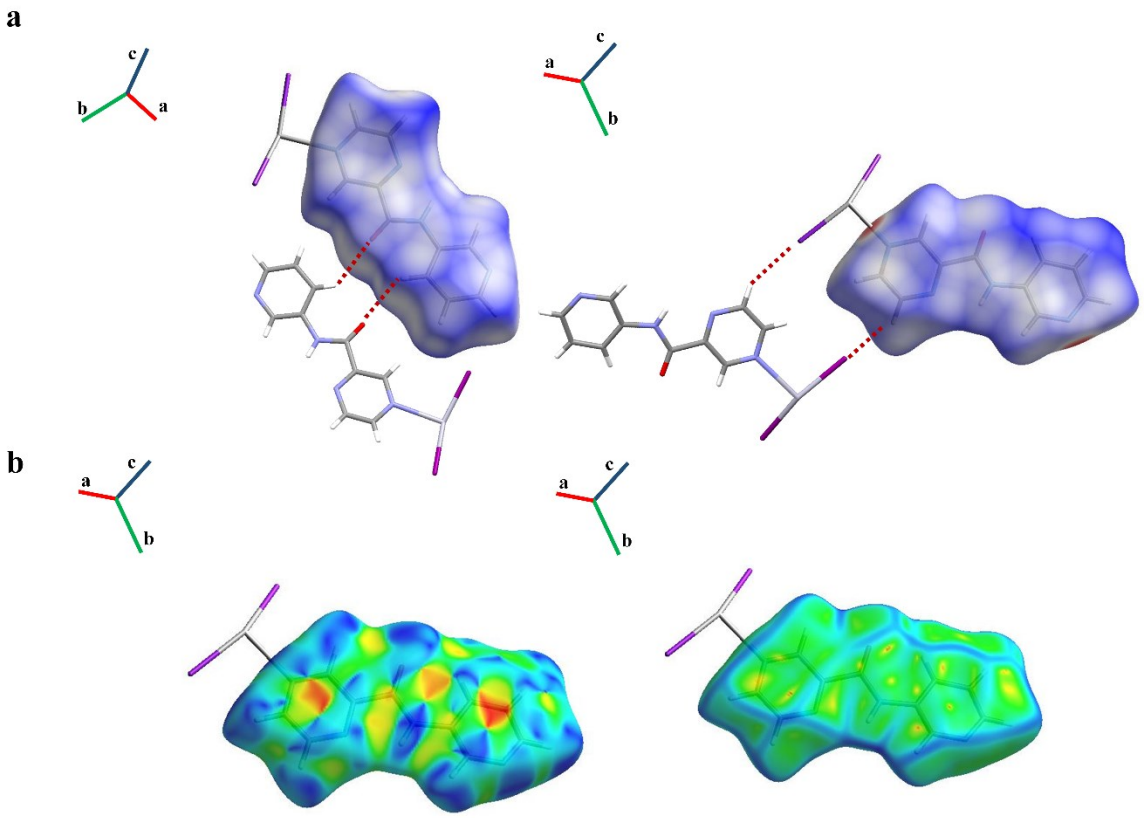

Figure S11. (a) Hirshfeld surface mapped with d_{norm}, showing C-H…O (left) and C-H…I (right) hydrogen bonds (b) Hirshfeld surface mapped with shape index (left) and curvedness (right) for compound 3.

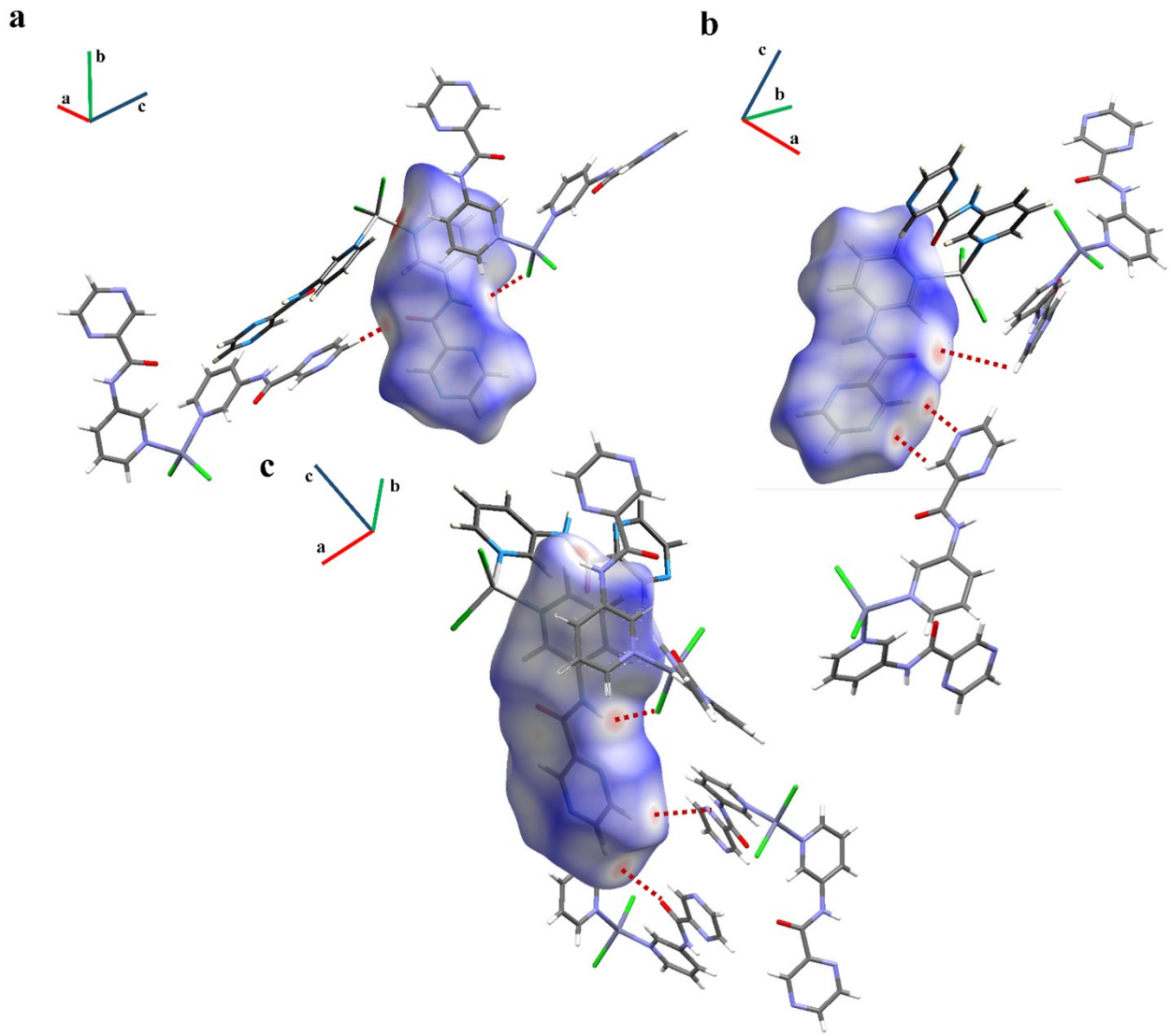

Figure S12. Hirshfeld surface mapped with d_{norm}, showing (a) C19-H19…O1 and N2-H2N…Cl1, (b) C10H10…O2, C18H18…N7 (c) N6H6N…Cl1, C20H20…N4, C19H19…O1 hydrogen bonds for compound 4.

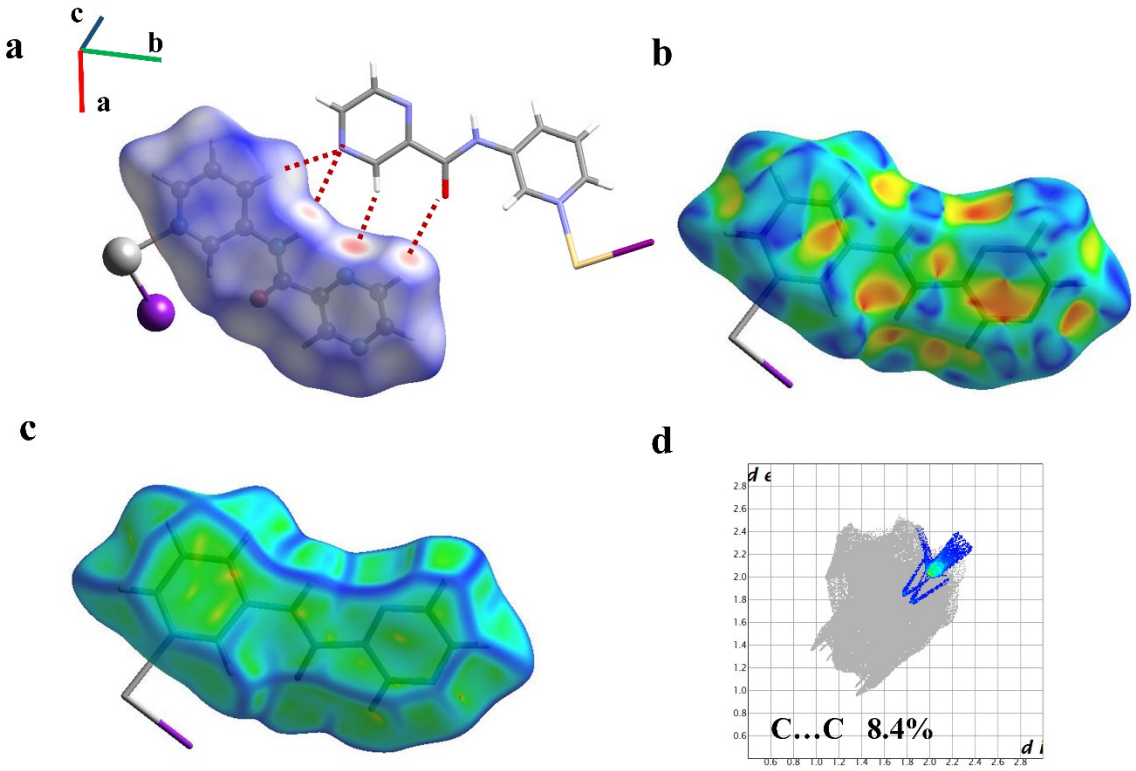

Figure S13. Hirshfeld surface mapped with (a) d_{norm}, showing C-H…O, C-H…N, N-H…N hydrogen bonds (b) shape index (c) curvedness and (d) decomposed finger print plots to C-C contacts for compound **5**.

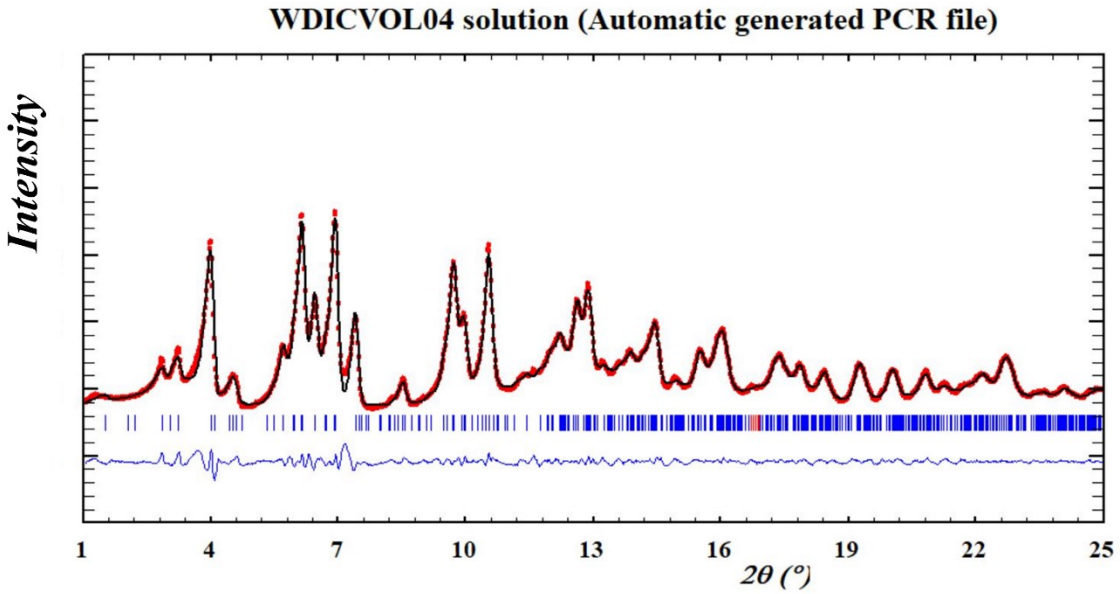

Figure 14. View of the best-fit profile of the Rietveld refinement of compound **6**

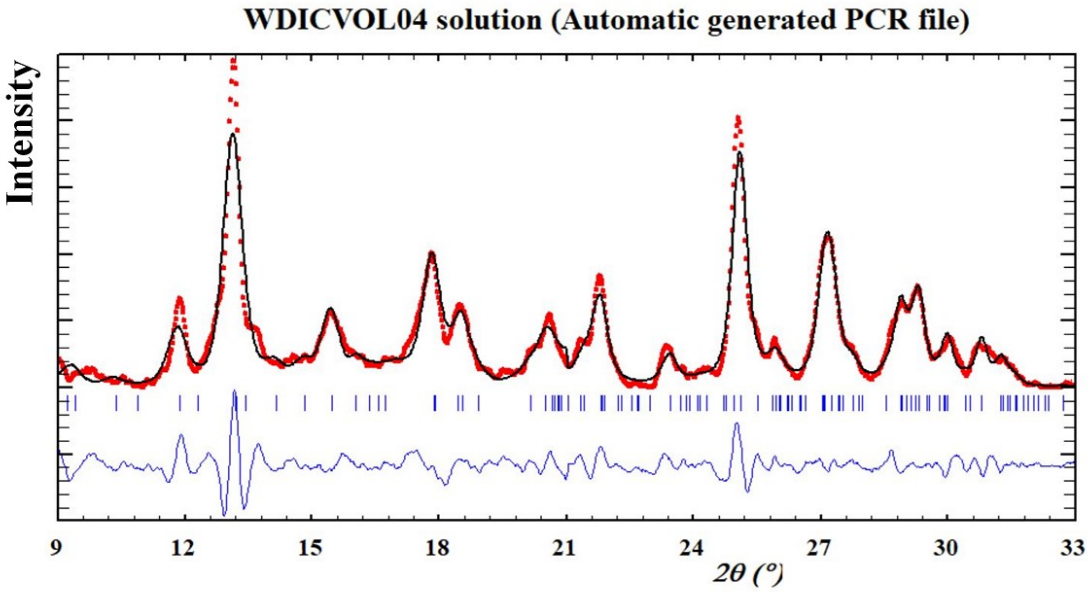

Figure S15. View of the best-fit profile of the Rietveld refinement of compound **9**

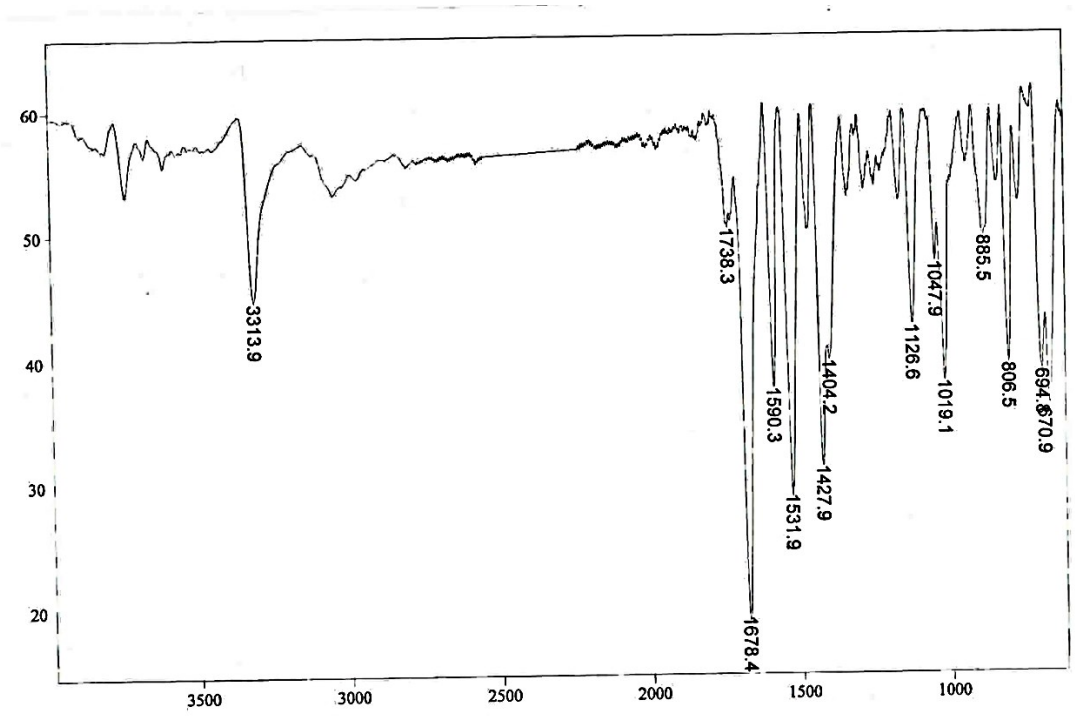

Fig. S16 IR Spectrum of ligand

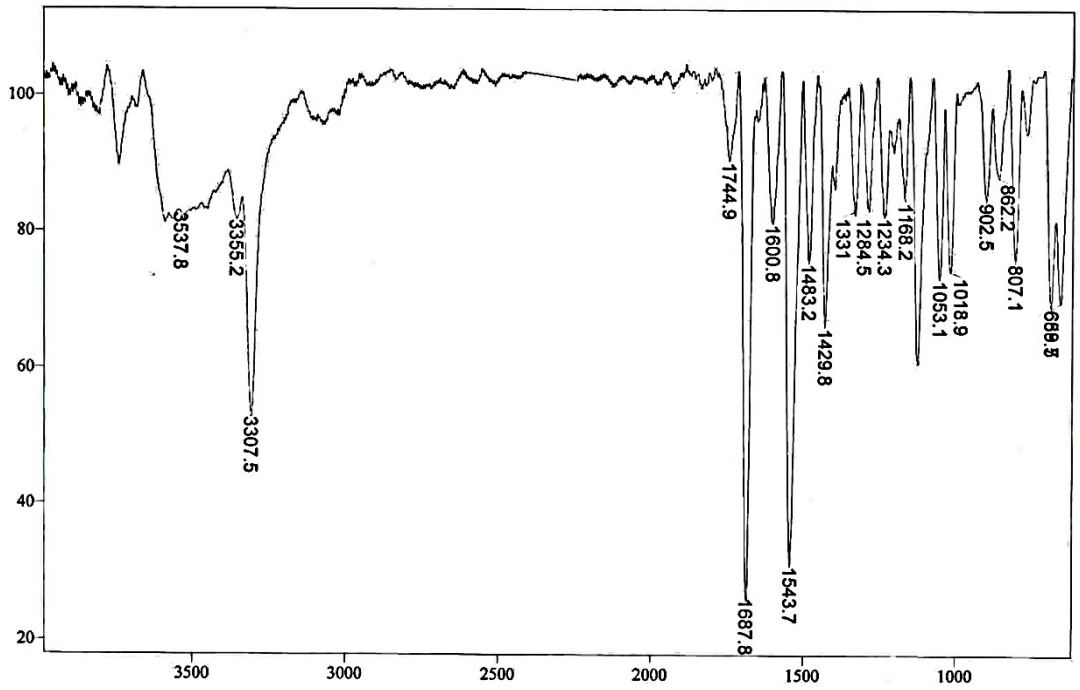

Fig. S17 IR Spectrum of compound **1**

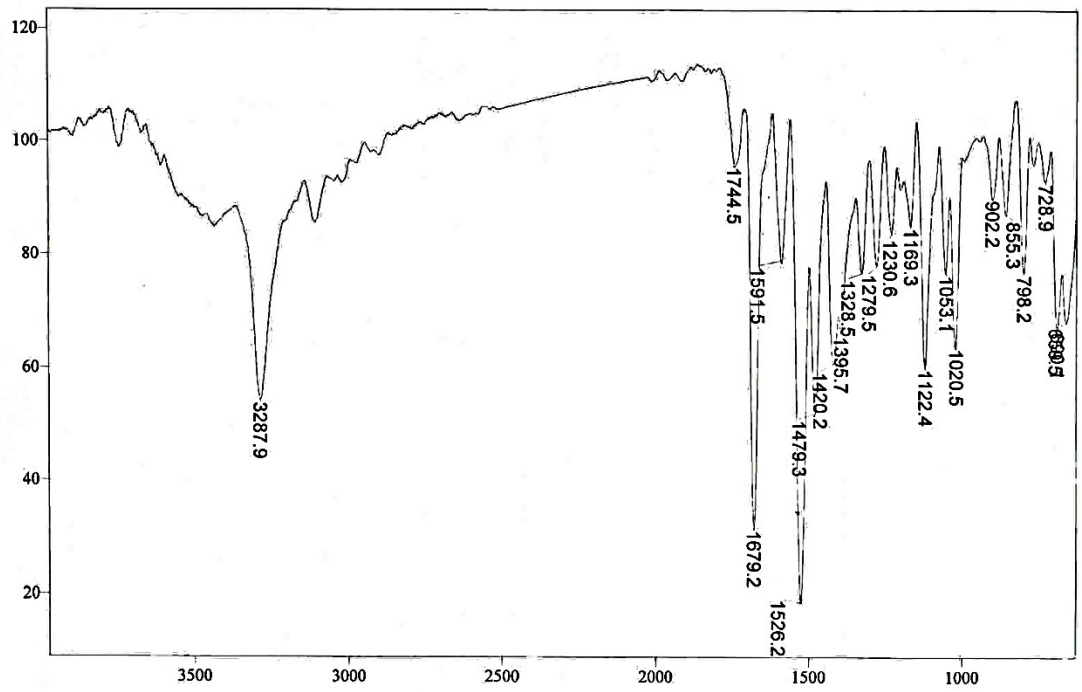

Fig. S18 IR Spectrum of compound **2**

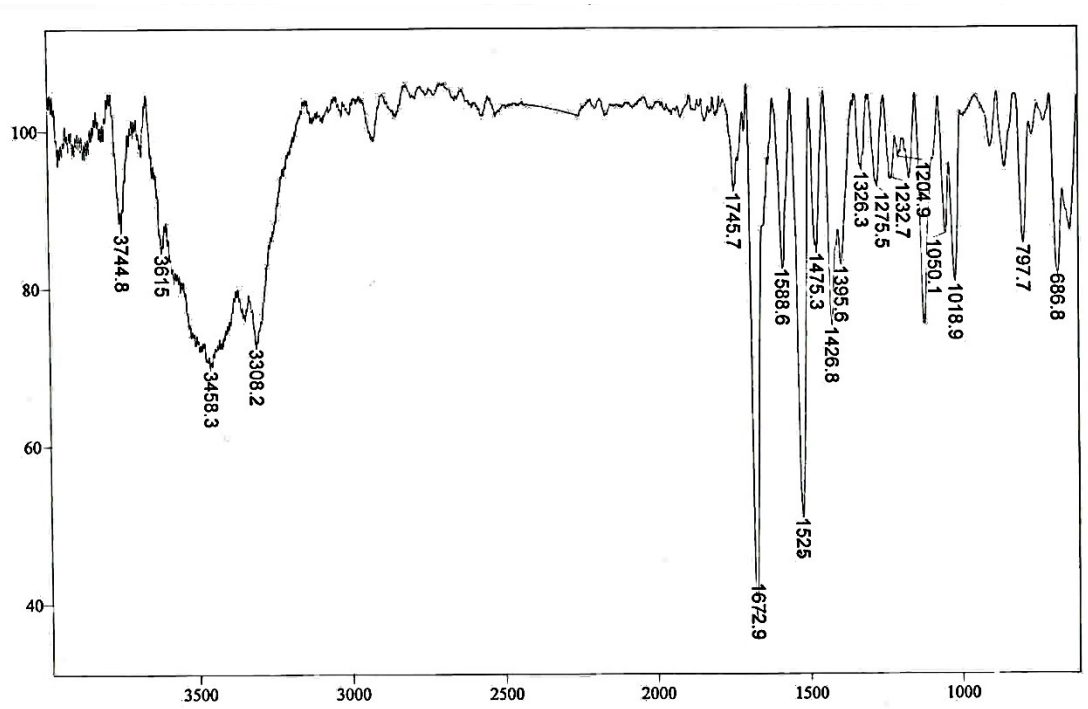

Fig. S19 IR Spectrum of compound **3**

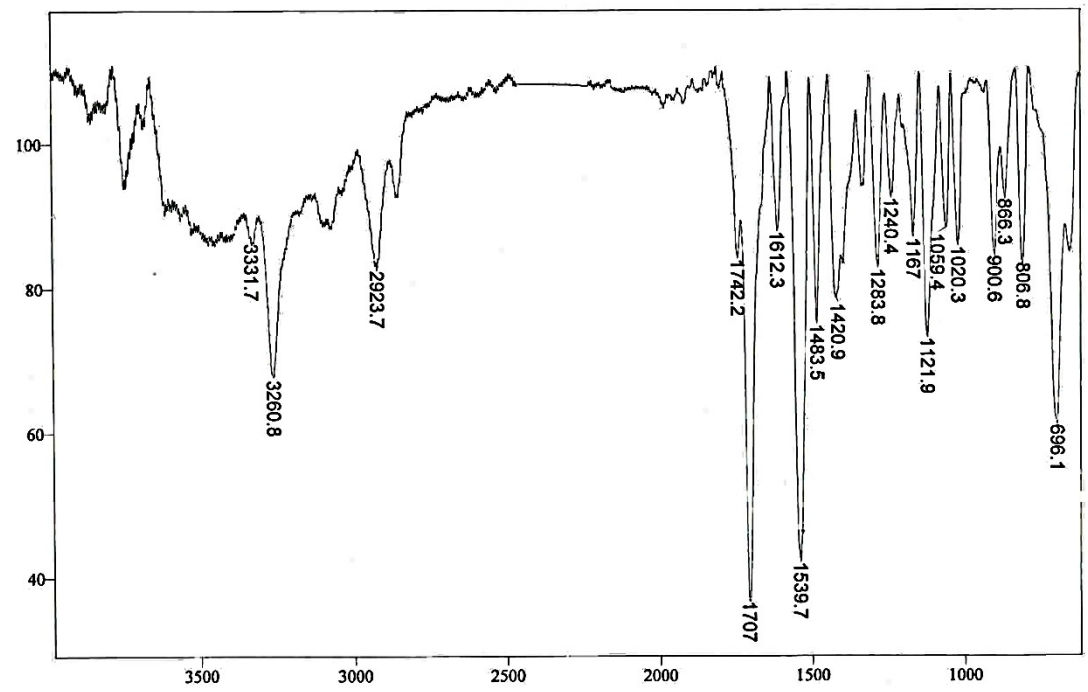

Fig. S20 IR Spectrum of compound **4**

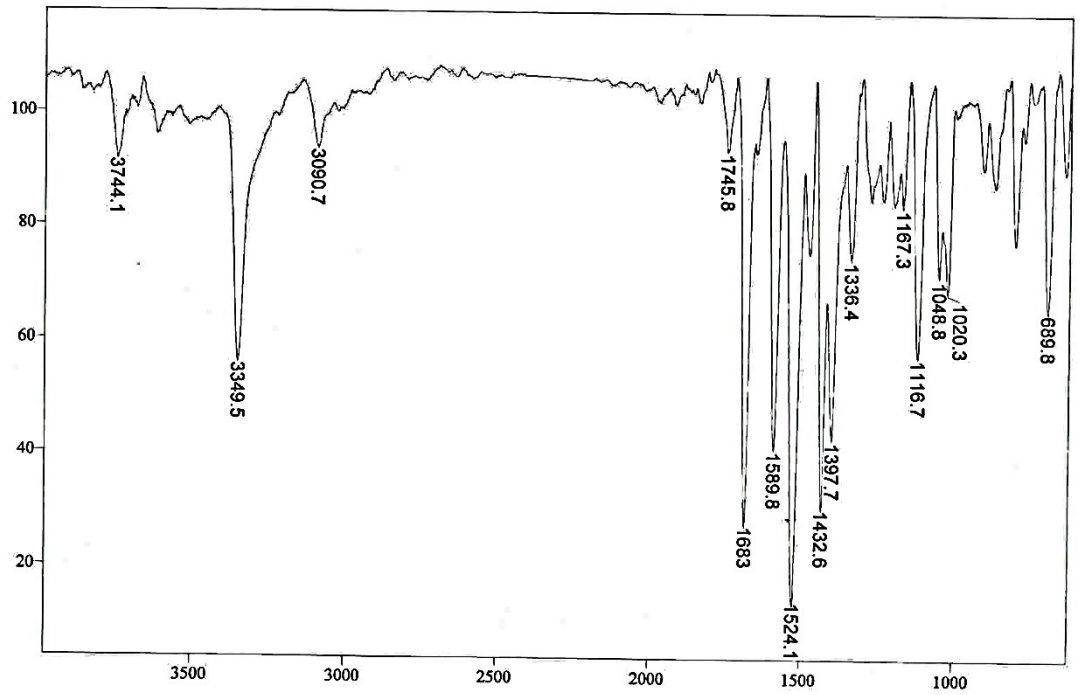

Fig. S21 IR Spectrum of compound **5**

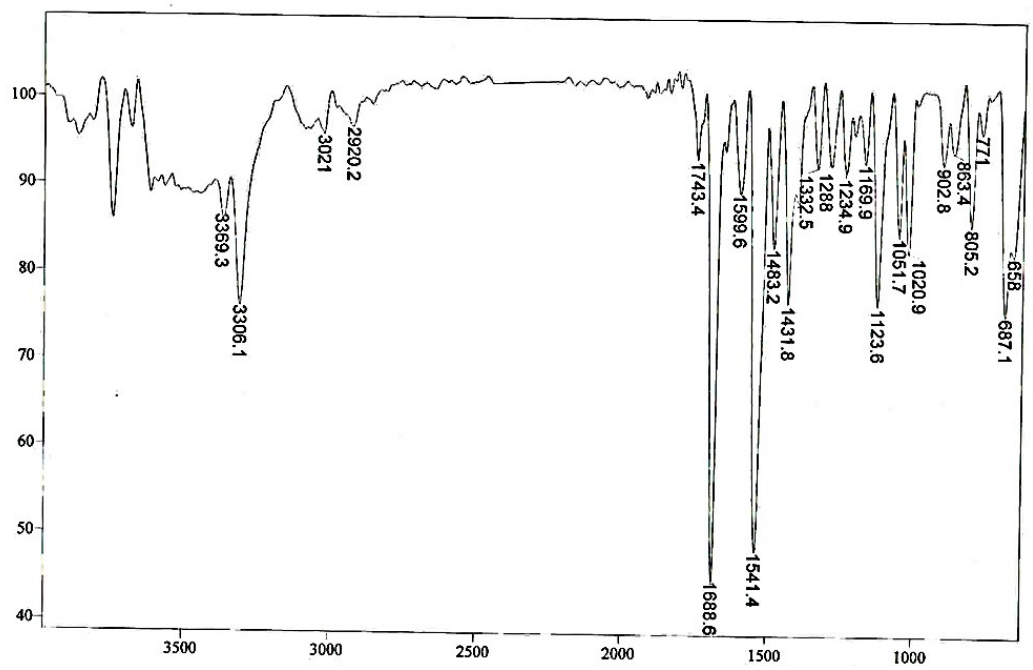

Fig. S22 IR Spectrum of compound **6**

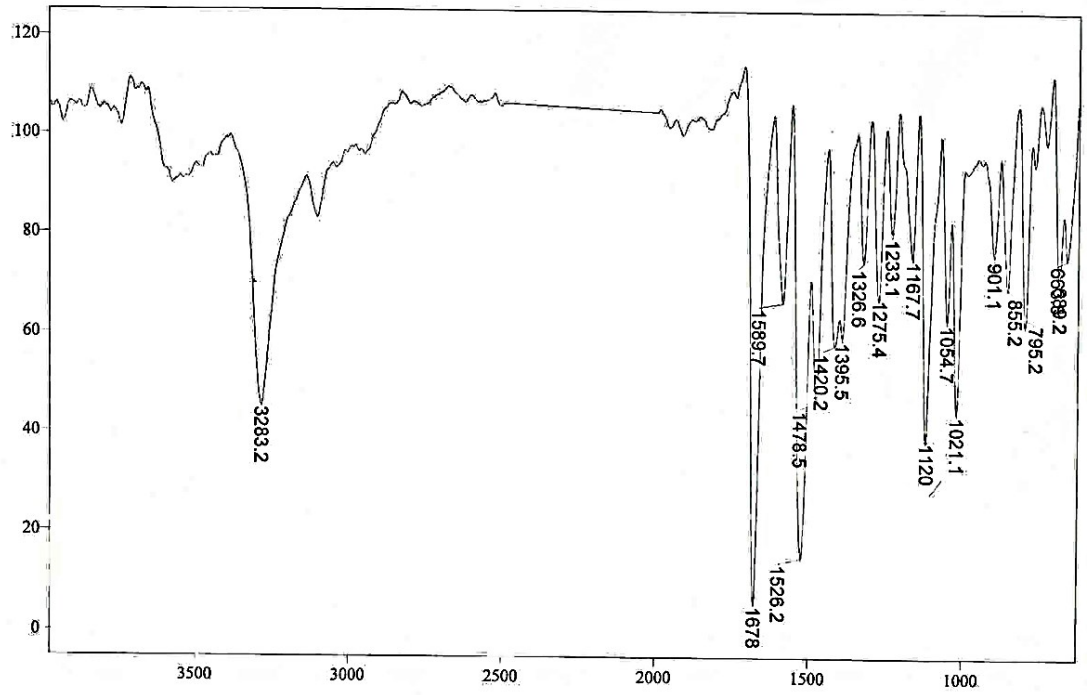

Fig. S23 IR Spectrum of compound **7**

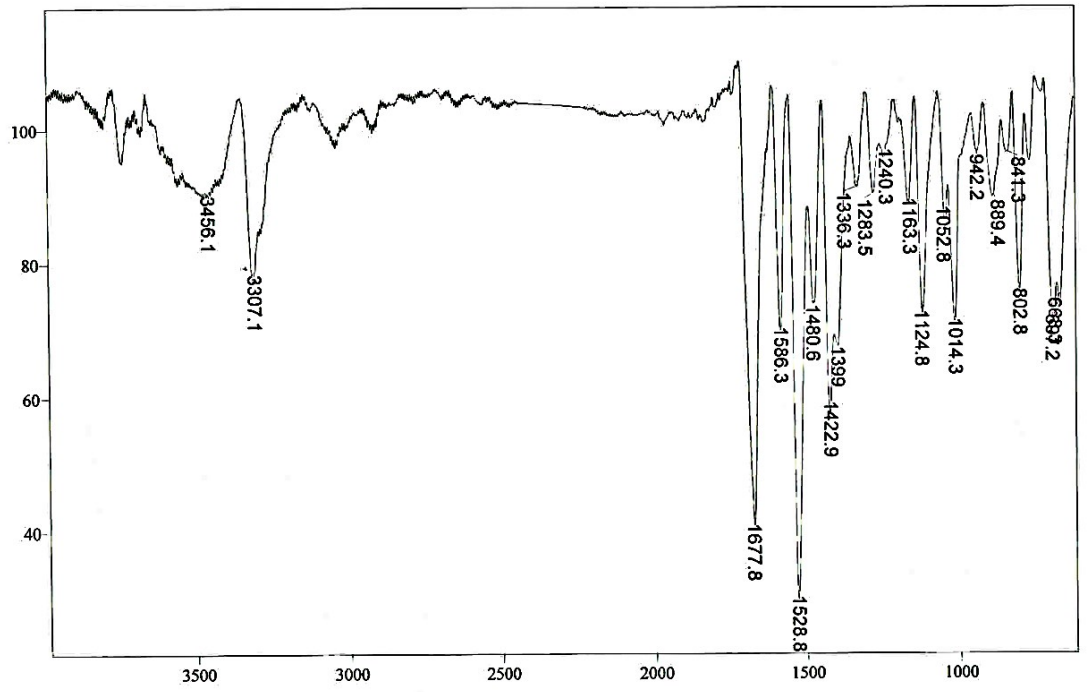

Fig. S24 IR Spectrum of compound **8**

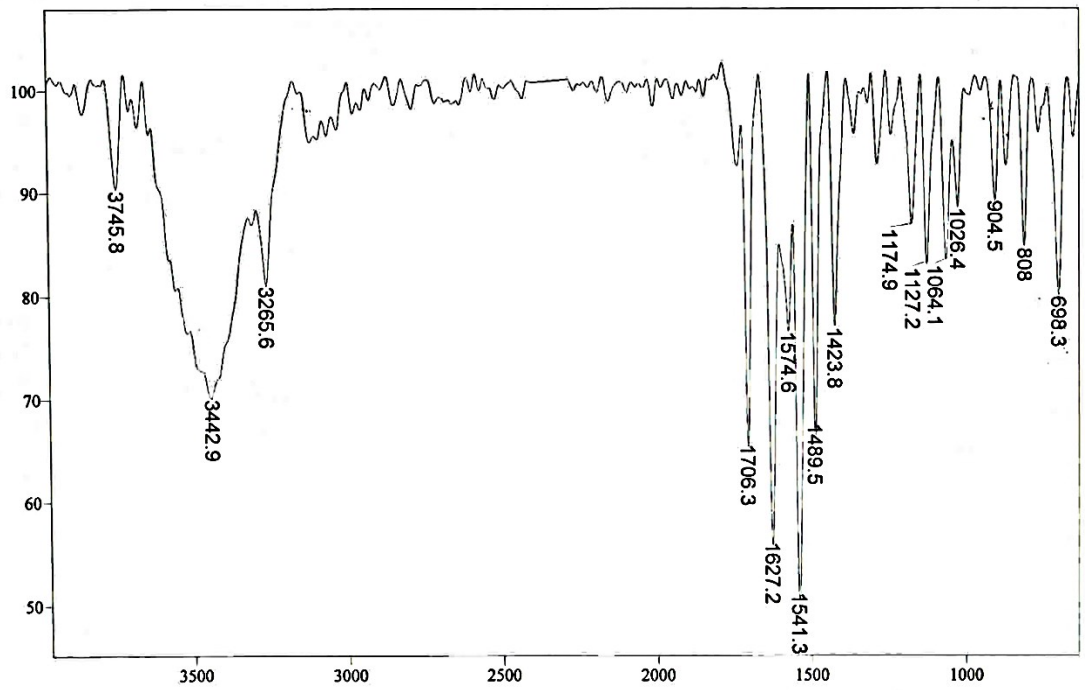

Fig. S25 IR Spectrum of compound **9**

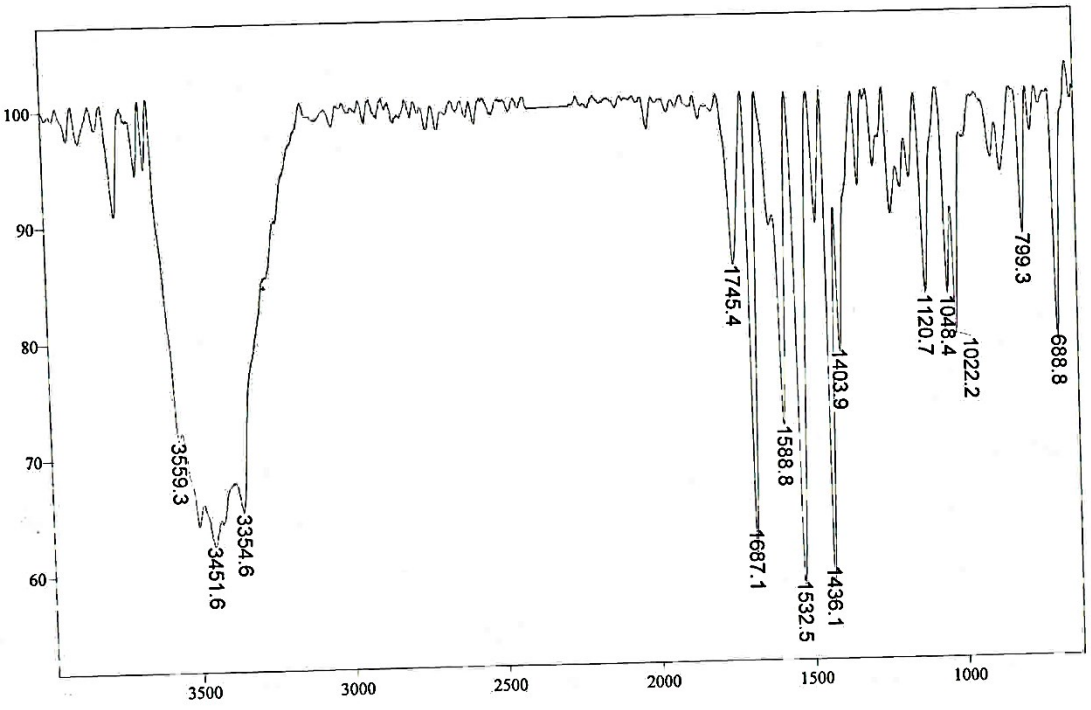

Fig. S26 IR Spectrum of compound **10**

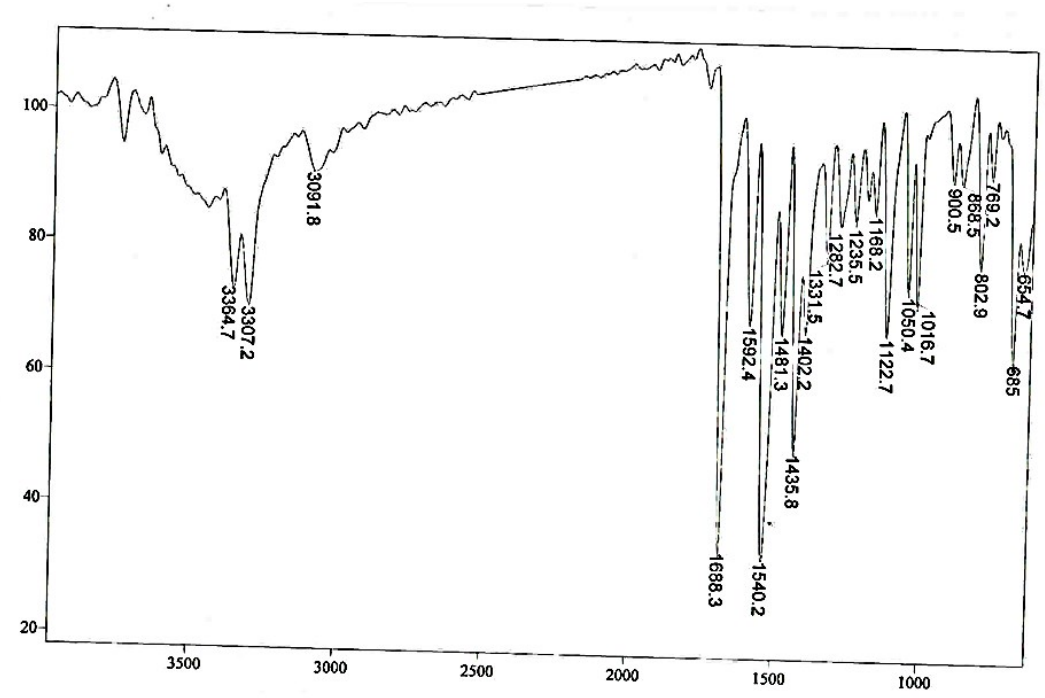

Fig. S27 IR Spectrum of compound **11**

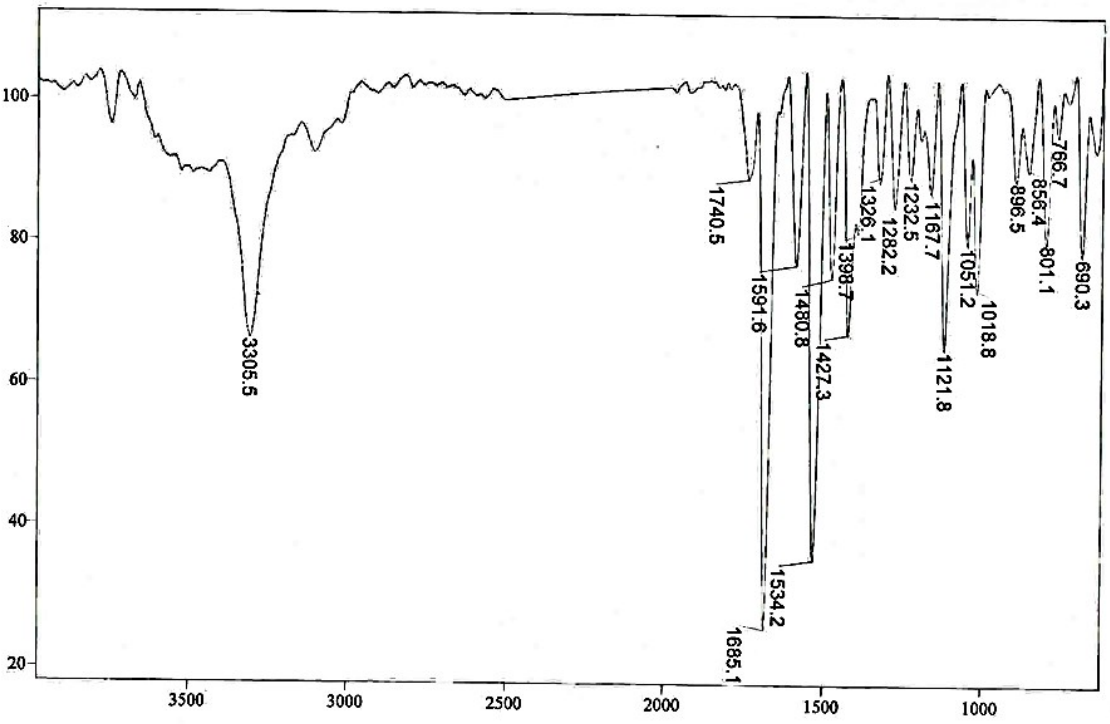

Fig. S28 IR Spectrum of compound **12**

References

1- M. Alfonso and H. Stoeckli-Evans, *ActaCryst.*, 2016, E72, 1214–1218.

2- H. R. Khavasi and B. Mir Mohammad Sadegh, *Inorg. Chem*., 2010, **49**, 5356–5358.

3- H. R. Khavasi, M. M. Barforoush and M. A. Fard, *CrystEngComm*., 2012, **14**, 7236-724.

4- H. R. Khavasi and A. A. Tahrani, *CrystEngComm,* 2013, **15**, 5799-5812.

5- H. R. Khavasi and M. Azizpoor Fard, *Cryst. Growth Des.*, 2010, **10**, 1892-1896.

6- H-J. Holdt, H. Muller, A. Kelling, H-J. Drexler, T. Muller, T.S chwarze, U. Schilde and I. Starke, *Z.Anorg.Allg.Chem.,* 2006, **632**, 114-122.

7- E-C. Yang, Y. Feng, Z-Y. Liu, T-Y. Liu and X-J. Zhao, *CrystEngComm*., 2011, 13, 230-242.

8- H. R. Khavasi and S. Kavand , *CrystEngComm.,* 2016, **18**, 4760-4764.

9- B. Notash, N. Safari, and H .R. Khavasi, *Inorg.Chem*. 2010, **49**, 11415-11420.

10- P. Nockemann and G. Meyer, *Acta Cryst*., 2004. **E60**, m744-m746.

11- Y-W. Li , Y. Tao , L-F. Wang , T-L. Hu and X-H. Bu, *RSC Adv*., 2012, **2**, 4348-4352.

12- L. Zhang, X-H. Zhao and Y. Zhao, *Acta Cryst*., 2005, **E61**, m1760–m1761.

13- C-W. Yeh, U. Ray and J-D. Chen, *J.Chin.Chem.Soc.,(Taipei)*2009, **56**, 1216-1224.

14- H. R. Khavasi and B. Mir Mohammad Sadegh, *Dalton Trans*., 2015, 44, 5488-5502.

15- H. R. Khavasi, A. R. Salimi, H. Eshtiagh-Hosseini and M. M. Amini, *CrystEngComm.*, 2011, 13, 3710-

16-Y. Qiu, B. Liu, G. Peng, J. Cai, H. Deng and M. Zeller, *Inorg. Chem. Commun.,* 2010, **13**, 749–752.

17- H. Khavasi and A. Azhdari Tehrani*, Inorg. Chem*., 2013, **52**, 2891–2905.

18- M. Nolte, I. Pantenburg and G. Meyer, Z.Anorg.Allg.Chem. (2008), 634, 362-368.

19- G. Mahmoudi and A. Morsali, *CrystEngComm* (2009), **11**, 1868 1868-1879.

20- C. Slabbert and M. Rademeyer, *CrystEngComm*., 2015, **17**, 9070-9096.

21- A. Azhdari Tehrani, B. Mir Mohammad Sadegh and H. R. Khavasi, *Acta Crystallogr.,Sect.E:Struct.Rep.Online*., 2010, **66**, m261-

22- J. R. Allan, A. D. Paton, A. J. Blake and K. Turvey, *Acta Crystallogr.,Sect.C:Cryst.Struct.Commun.,*1989, **45**, 1422-1424.

23- H. R. Khavasi and B. M. M. Sadegh, *Dalton Trans*., 2014, **43**, 5564-5573.

24- Y-B. Dong, M. D. Smith and H-C zur Loye, *Solid State Sciences*., 2000, **2**, 861–870.

25- S. Kasselouri, A. Garoufis, S. Paschalidou, S. P. Perlepes, I. S. Butler and N. Hadjiliadis, *Inorg.Chim.Acta*., 1994, **227**, 129-136.

(2015), **190**, 360

26- A. Dadrass, H. Rahchamani, J. Khalafy, A. Ramazani, B. P. Habashi, A. P. Marjani, A. Souldozi, K. Slepokura, T. Lis and M. Rouhani, *Sulfur, Silicon, Relat.Elem.,*2015, 190, 360-371.

27- Q. Zhao, Z. Shen, H. Yang, Q. Zhou and Q-H. Wang, *Jiegou Huaxue.,* 2016, **35**, 1253-1259.

28- H. R. Khavasi, F. Norouzi and A. A. Tehrani, *Cryst.Growth Des*., 2015, **15**, 2579-2583.

29- A. P. Marjani, B. P. Habashi, H. Rahchamani, J. Khalafy, A. Dadrass and H. Y. Asl, *Jiegou Huaxue.,* 2014, **33**, 1460

30- Q. Zhao, Z. Shen, H. Yang and H-Z. Song, *Jiegou Huaxue.,* 2016, **35**, 69-76.

31- B. Mir Mohammad Sadegh, A. Azhdari Tehrani and H. R. Khavasi, *Acta Crystallogr.,Sect.E:Struct.Rep.Online.,* 2010, **66**, m158.

32- P. Nockemann and G. Meyer, *Acta Crystallogr., Sect.E:Struct.Rep.Online*., 2004, **60**, m747-m748.

33- G-W. Wang, W-Y. Wu, L-H. Zhuang and J-T. Wang, *Acta Crystallogr.,Sect.E:Struct.Rep.Online.,* 2008, **64**, m13.

34- J-Y. Wu, H-Y. Hsu, C-C. Chan, Y-S. Wen, C. Tsai and K-L. Lu, *Cryst.Growth Des.* 2009, **9**, 258-262.

35- C. Slabbert and M. Rademeyer, *CrystEngComm.,* 2016, **18**, 4555-4579.

36- J-L. Du, Z-Z. Wei and T-L. Hu, *Solid State Sciences.,* 2011, **13**, 1256-1260.

37- S. P. Perlepes, S. Kasselouri, A. Garoufis, F. Lutz, R. Bau, and N.Hadjiliadis, *Polyhedron.* 1995, **14**, 1461-1470.

38- F. Yu, W. Zhang, P. Li, Y. Xing, L. Tong, J. Ma and B.Tang, *The Analyst*., 2009, **134**,1826-1833.

39- P. Nockemann and G. Meyer, *Acta Crystallogr.,Sect.E:Struct.Rep.Online*., 2004, E **60**, m749-m750.

40- L. Saghatforoush*, Jiegou Huaxue*., 2015, **34**, 1869- 1875.

41- O. Vallat, A. Neels and H. Stoeckli-Evans, *J.Chem.Cryst*., 2003, 33, 39-50.

42-S. A. Shirvan, M. R. Asghariganjeh, M. Aghajeri, S. Haydari Dezfuli and F. Hossini, *Acta Crystallogr.,Sect.E:Struct.Rep.Online.,* 2012, 68, m303-m309.

43- Y-B. Dong, M. D. Smith and H-C.zur Loye, *Angew.Chem.,Int.Ed.*, 2000, **39**, 4271-4273.

44- A. Garoufis, S. P. Perlepes, A. Schreiber, R. Bau and N. Hadjiliadis, *Polyhedron*., 1996, **15**, 177-182.