Distinguishable Zn(II) and Pb(II) template effects on forming pendant-armed Schiff-base macrocyclic complexes including a unprecedented Pb(II)–π macrocyclic complex

Kun Zhang, Jiao Geng, Chao Jin and Wei Huang

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Table SI1 Selected bond distances (Å) and angles (°) in **1–4**.

Bond distances		Bond angles	
1a·C_2H_5OH			
Zn1–O1	1.953(3)	O1–Zn1–O2	97.6(1)
Zn1–O2	1.981(3)	O1–Zn1–O7	104.8(1)
Zn1–O7	2.178(3)	O1–Zn1–N1	90.0(1)
Zn1–N1	2.088(3)	O1–Zn1–N2	125.6(1)
Zn1–N2	2.046(3)	O2–Zn1–O7	90.7(1)
Zn2–O3	1.970(3)	O2–Zn1–N1	171.4(1)
Zn2–O4	2.008(3)	O2–Zn1–N2	92.7(1)
Zn2–O7	2.093(3)	O7–Zn1–N1	83.4(1)
Zn2–N3	2.121(3)	O7–Zn1–N2	128.5(1)
Zn2–N4	2.047(4)	N1–Zn1–N2	86.1(1)
		O3–Zn2–O4	92.5(1)
		O3–Zn2–O7	110.2(1)
		O3–Zn2–N3	87.3(1)
		O3–Zn2–N4	126.4(1)
		O4–Zn2–O7	87.8(1)
		O4–Zn2–N3	177.0(1)
		O4–Zn2–N4	91.1(1)
		O7–Zn2–N3	95.2(1)
		O7–Zn2–N4	123.4(1)
		N3–Zn2–N4	86.6(2)

		Zn1–O7–Zn2	126.2(1)
		Zn1–O7–N7	114.0(2)
		Zn2–O7–N7	112.5(2)
1b·CH_3OH			
Zn1–O1	1.979(5)	O1–Zn1–O4	97.2(2)
Zn1–O4	1.982(4)	O1–Zn1–O5	101.6(2)
Zn1–O5	2.125(4)	O1–Zn1–N5	143.1(2)
Zn1–N5	2.070(6)	O1–Zn1–N6	86.7(2)
Zn1–N6	2.113(6)	O4–Zn1–O5	92.1(2)
Zn2–O2	1.965(5)	O4–Zn1–N5	90.5(2)
Zn2–O3	2.012(4)	O4–Zn1–N6	174.0(2)
Zn2–O5	2.160(5)	O5–Zn1–N5	115.2(2)
Zn2–N2	2.080(6)	O5–Zn1–N6	93.8(2)
Zn2–N3	2.052(6)	N5–Zn1–N6	87.9(2)
		O2–Zn2–O3	95.5(2)
		O2–Zn2–O5	113.9(2)
		O2–Zn2–N2	90.1(2)
		O2–Zn2–N3	120.9(2)
		O3–Zn2–O5	88.0(2)
		O3–Zn2–N2	173.4(2)
		O3–Zn2–N3	91.5(2)
		O5–Zn2–N2	86.6(2)
		O5–Zn2–N3	125.0(2)
		N2–Zn2–N3	88.6(3)
		Zn1–O5–Zn2	124.5(2)
		Zn1–O5–N7	116.5(4)
		Zn2–O5–N7	110.7(4)
2			
Pb1–O1	2.283(4)	O1–Pb1–O2	75.6(1)
Pb1–O2	2.325(4)	O1–Pb1–N2	113.4(2)
Pb1–N2	2.519(5)	O1–Pb1–N3	74.1(2)
Pb1–N3	2.462(5)	O2–Pb1–N2	72.8(2)
Pb1–C26	3.468(10)	O2–Pb1–N3	111.6(2)
Pb1–C27	3.578(8)	N2–Pb1–N3	66.0(2)
Pb1–C25	3.708(10)		
Pb1–C22	3.946(7)		
Pb1–C24	3.991(10)		

Pb1–C23	4.102(8)		
3			
Pb1–O1	2.330(8)	O1–Pb1–N1	72.9(3)
Pb1–N1	2.503(10)	O1–Pb1–O1^{c}	74.8(3)
Pb1–O1^{c}	2.330(8)	O1–Pb1–N1^{c}	112.1(3)
Pb1–N1^{c}	2.503(10)	O2^{c}–Pb1–N1	112.1(3)
Pb1–O2^{c}	3.291(14)	N1–Pb1–N1^{c}	66.9(3)
		O2^{c}–Pb1–N1^{c}	72.9(3)
4			
Zn1–O1	2.112(5)	O1–Zn1–O2	87.4(2)
Zn1–O2	2.118(6)	O1–Zn1–O3	83.0(2)
Zn1–O3	2.319(5)	O1–Zn1–O1^{a}	81.3(2)
Zn1–O1^{a}	2.108(5)	O1–Zn1–O4^{a}	84.7(2)
Zn1–O4^{a}	2.044(5)	O1–Zn1–N1^{a}	171.1(2)
Zn2–N1^{a}	2.138(5)	O2–Zn1–O3	89.8(2)
		O1^{a}–Zn1–O2	164.9(2)
		O2–Zn1–O4^{a}	92.9(2)
		O2–Zn1–N1^{a}	101.5(2)
		O1^{a}–Zn1–O3	79.0(2)
		O3–Zn1–O4^{a}	167.2(2)
		O3–Zn1–N1^{a}	97.0(2)
		O1^{a}–Zn1–O4^{a}	96.0(2)
		O1^{a}–Zn1–N1^{a}	90.0(2)
		O4^{a}–Zn1–N1^{a}	94.8(2)
		Zn1–O1–Zn1^{a}	98.7(2)

Symmetry codes: ^{a}, 2–*x, –y,* 1–*z*; ^{c}, *x, –y, z*.

Table SI2 Hydrogen bonding parameters (Å, °) in **1–4**.

D–H···A	D–H	H···A	D···A	∠DHA	Symmetry code
1a·C_2H_5OH					
O1–H1···N5	0.93	2.19	2.804(4)	122	
O3–H3A···N5	0.93	1.95	2.682(4)	134	
O5–H5A···O12	0.82	1.97	2.696(8)	147	-1+*x*, -1+*y*, *z*
O6–H6···O10	0.82	2.03	2.764(6)	150	2-*x*, 1-*y*, -*z*
1b·CH_3OH					
O2–H2A···O1	0.97	2.50	3.141(6)	123	
O2–H2A···N1	0.97	1.95	2.767(7)	140	
O4–H4A···N4	0.97	2.03	2.807(7)	135	
3					
O1–H1A···N2	0.85	2.05	2.797(14	146	
4					
O3–H3A···O4	0.97	1.81	2.754(7)	164	

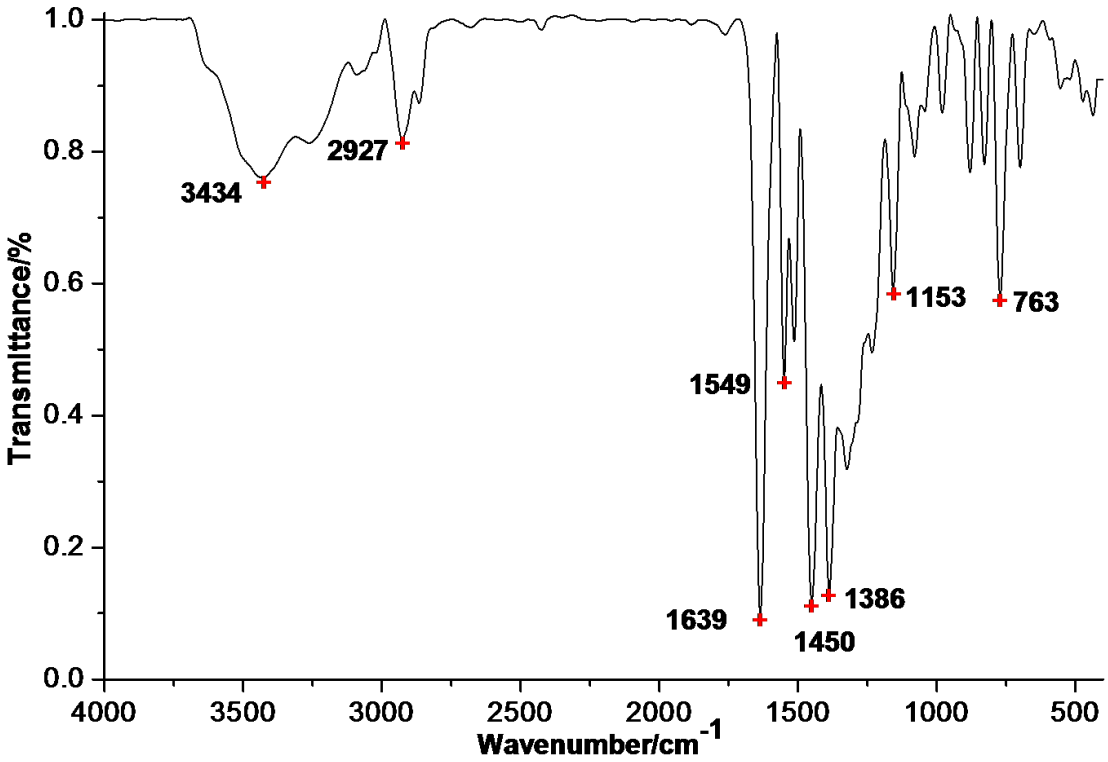

Figure SI1. FT–IR spectrum of Zn(II) complex **1a**.

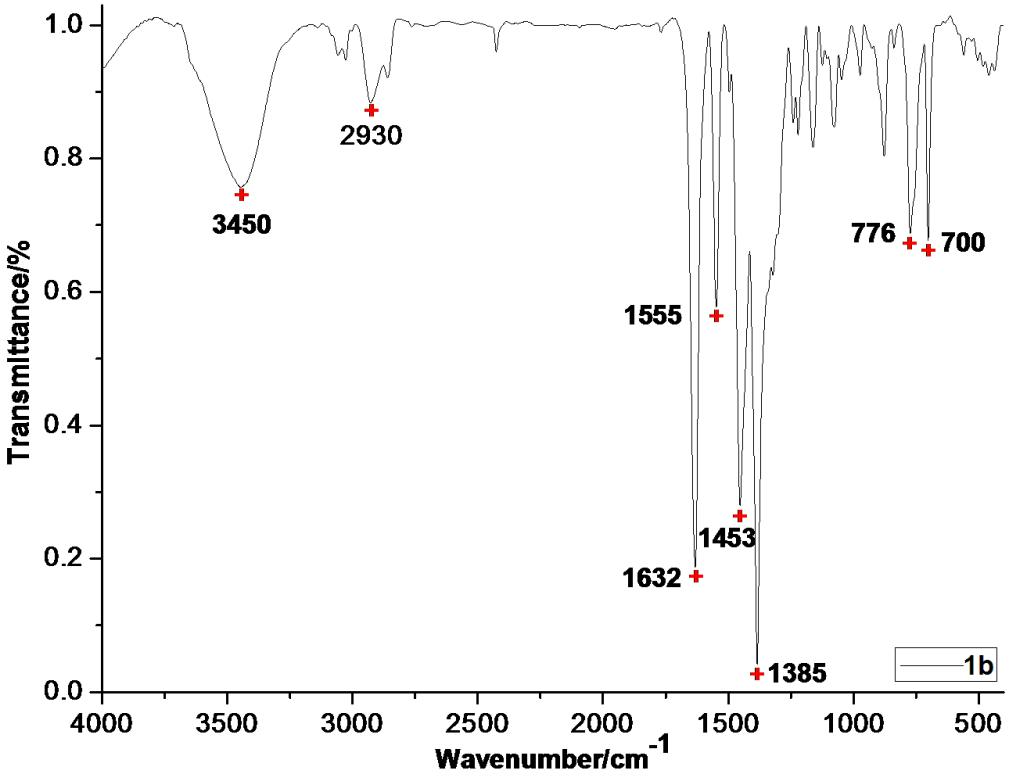

Figure SI2. FT–IR spectrum of Zn(II) complex **1b**.

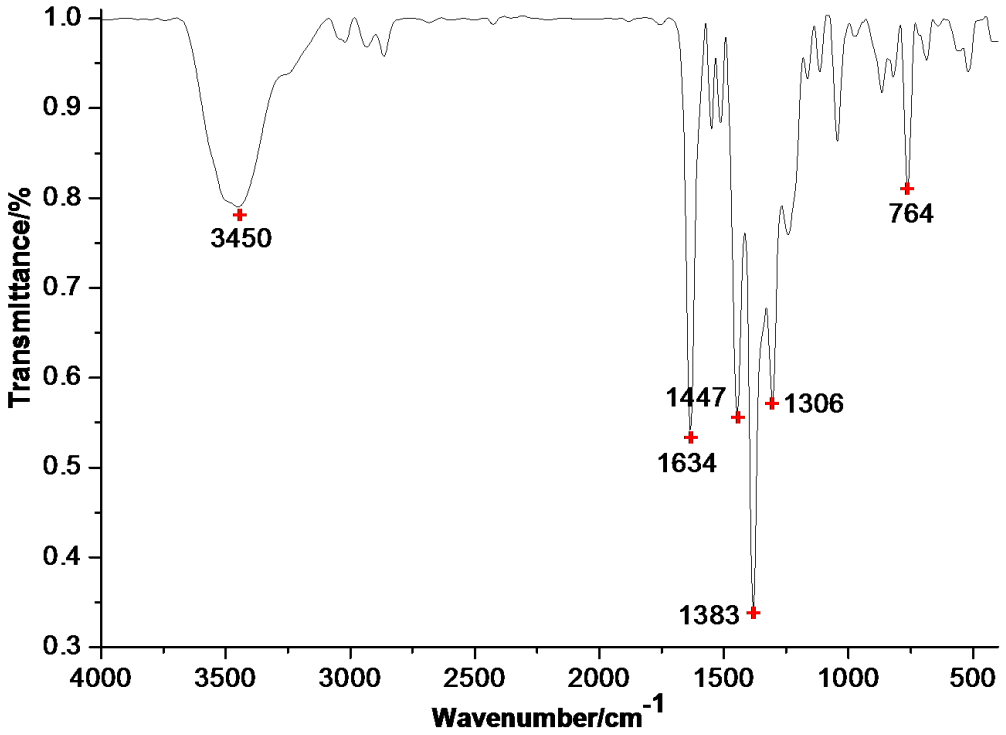

Figure SI3. FT–IR spectrum of Pb(II) complex **2**.

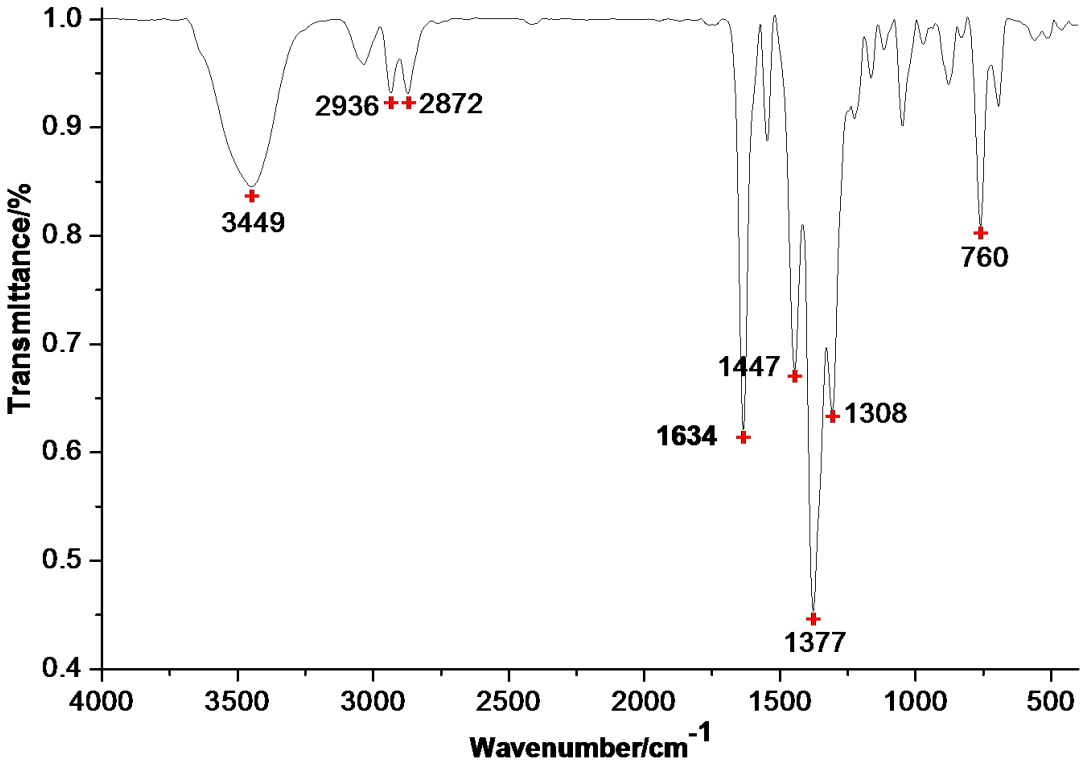

Figure SI4. FT–IR spectrum of Pb(II) complex **3**.

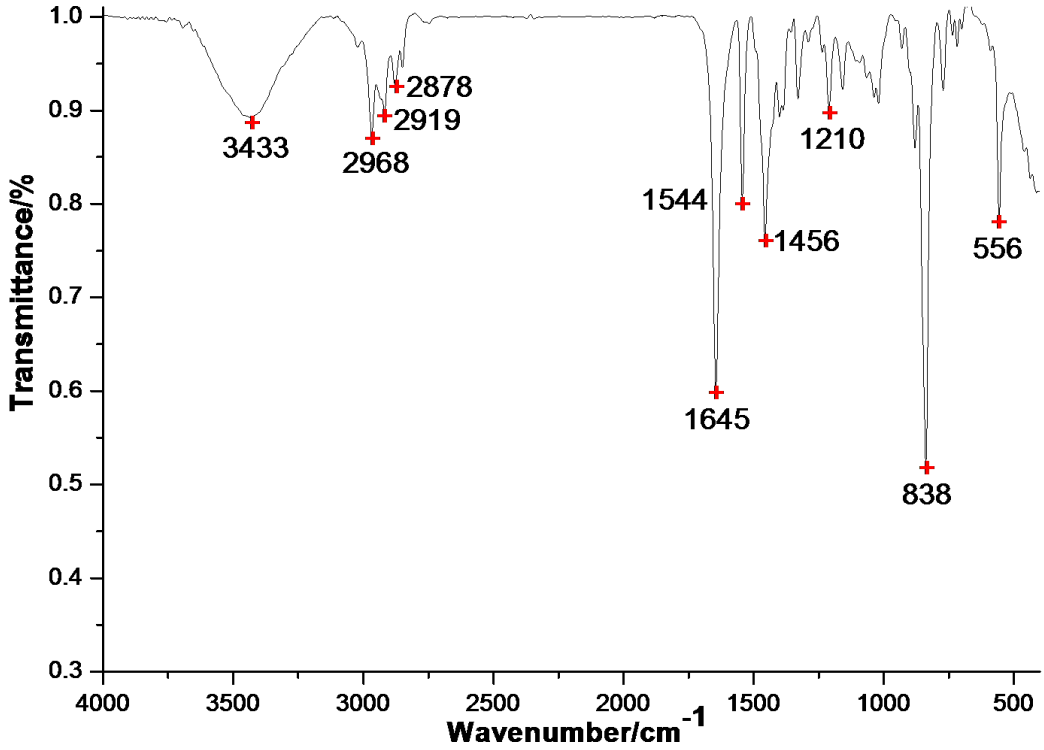

Figure SI5. FT–IR spectrum of Zn(II) complex **4**.

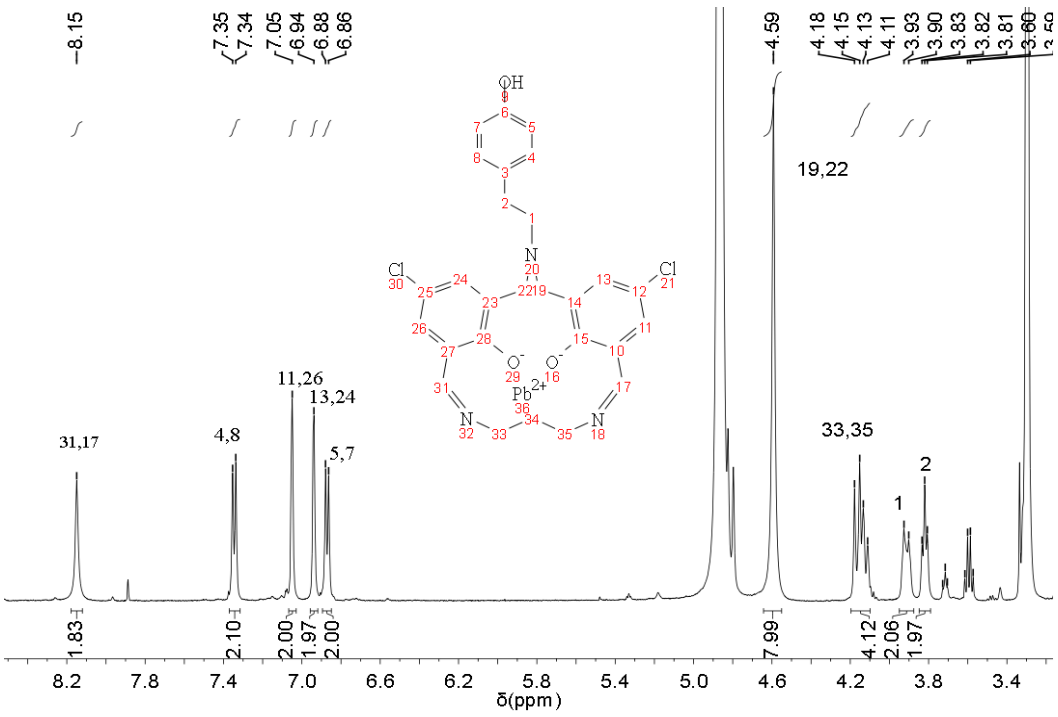

Figure SI6. ^{1}H NMR spectrum of Pb(II) complex **2** in CD_3OD.

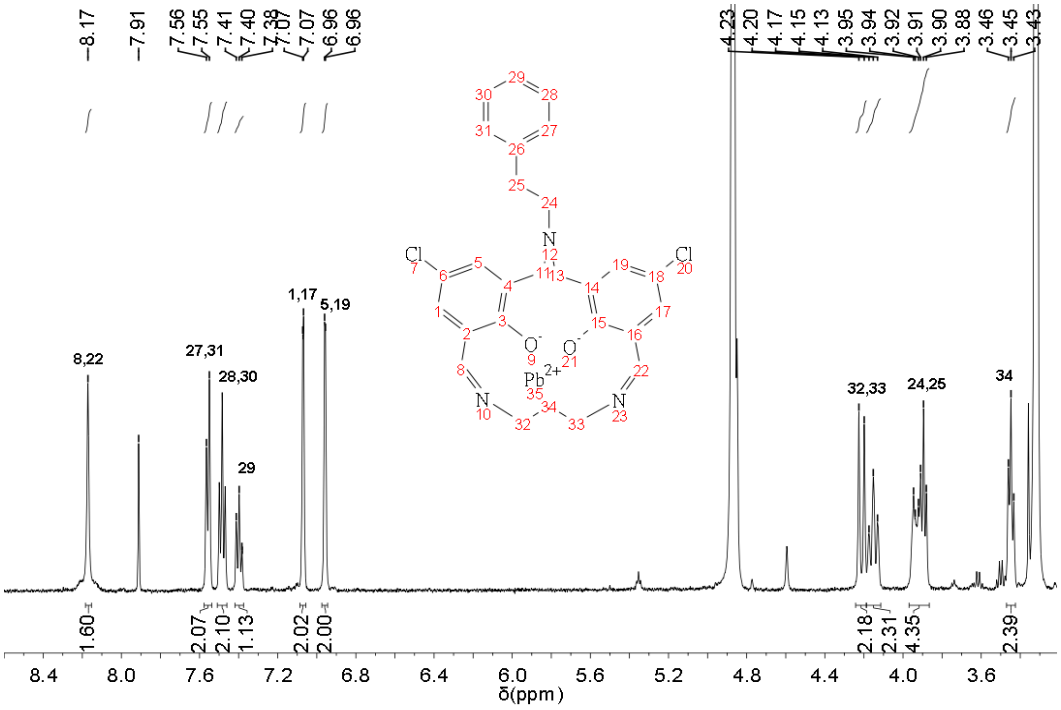

Figure SI7. ^{1}H NMR spectrum of Pb(II) complex **3** in CD_3OD.

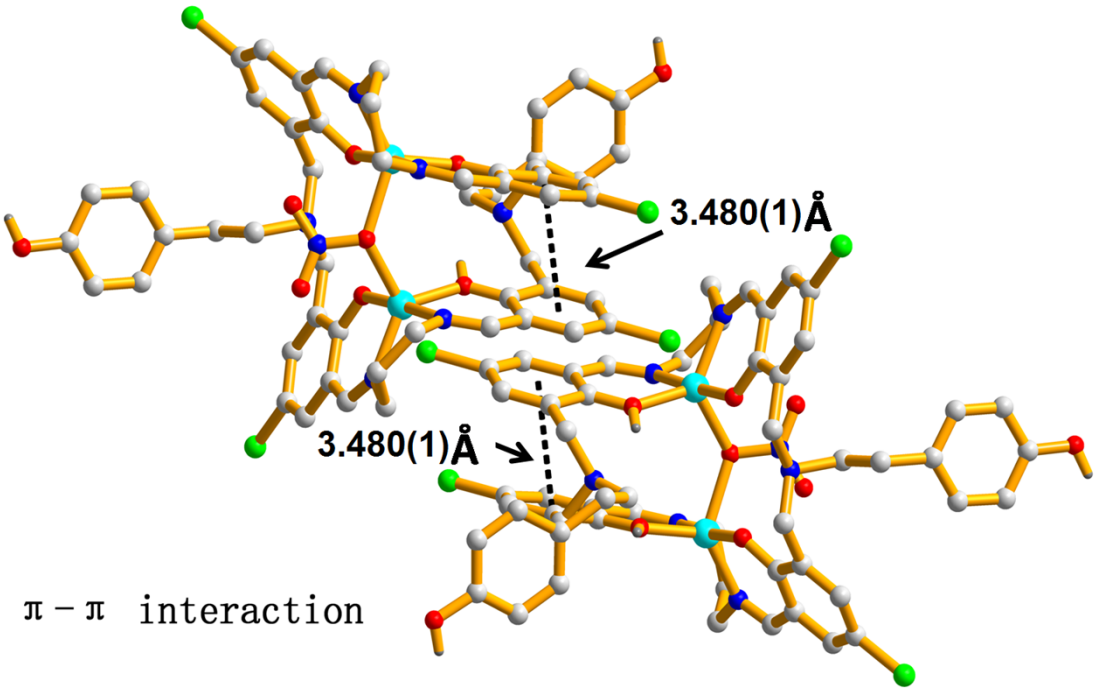

Figure SI8 Perspective view of the packing structure of compound **1a**·C_2H_5OH showing typical π–π stacking interactions.

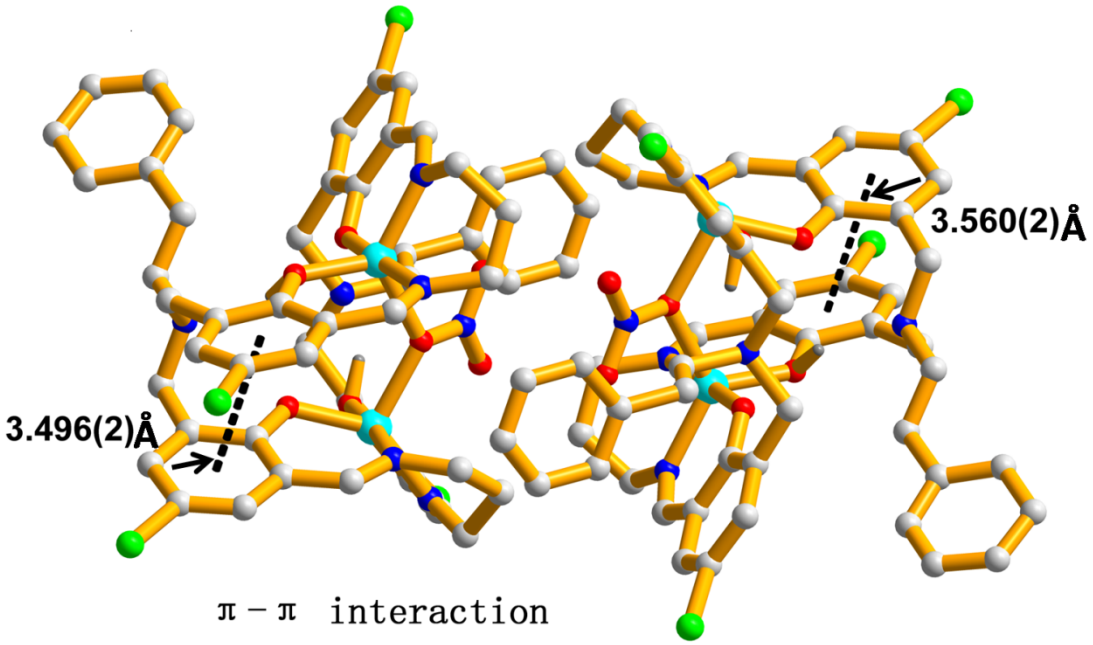

Figure SI9 Perspective view of the packing structure of compound **1b**·CH_3OH showing typical π–π stacking interactions.

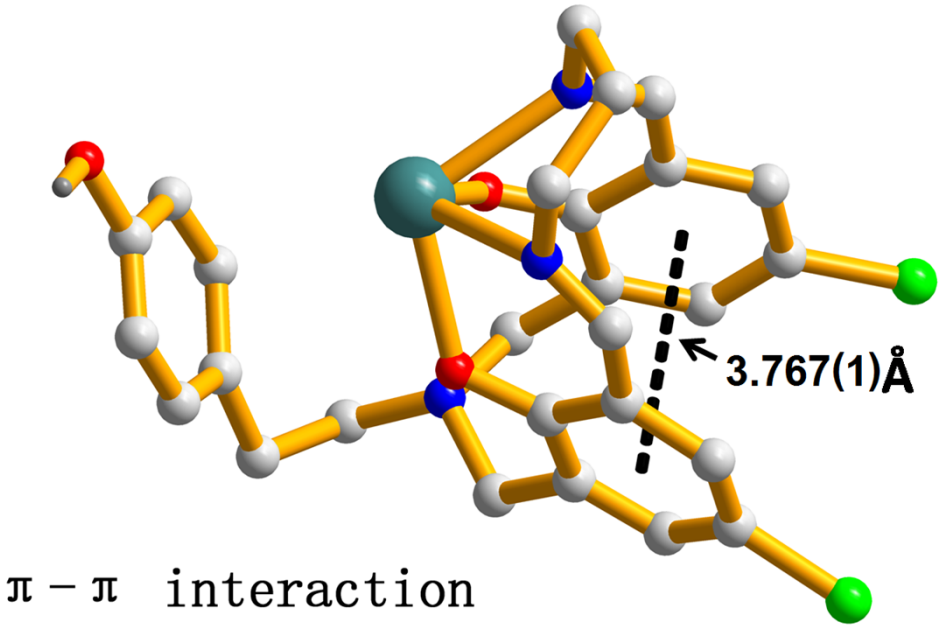

Figure SI10 Perspective view of the packing structure of compound **2** showing typical π–π stacking interactions.

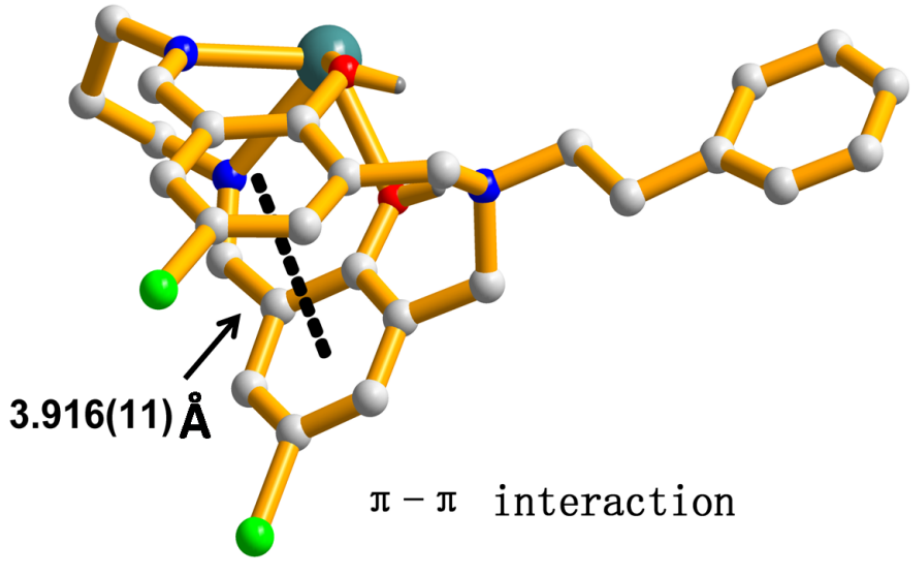

Figure SI11 Perspective view of the packing structure of compound **3** showing typical π–π stacking interactions.