Supporting Information

Crystallographic Insight into the Binding Modes of Group 12 Metal Cations with N7-Alkylated Purines

Subhra Jyoti Panda[1,2],‡ *Suraj Kumar Agrawalla*[1,2],‡ *Chandra Shekhar Purohit*[1,2]*

[1]School of Chemical Sciences, National Institute of Science Education and Research (NISER),

[2]An OCC of HBNI, Bhubaneswar, 752050, Odisha, India.

‡ Both authors contributed equally to the work.

E-mail: purohit@niser.ac.in,

Table of Contents

1 Material and Methods

1.1 General Experimental:

All the chemicals were purchased from Sigma-Aldrich, SRL Chemicals, and Spectrochem and used without further purification. All the solvents were dry distilled before use according to the standard procedures. Nuclear magnetic resonance spectra (^{1}H NMR and ^{13}C NMR) were recorded at Bruker AV-400 (^{1}H at 400 MHz and ^{13}C at 100 MHz) spectrometers. NMR chemical shifts were referenced in parts per million (ppm) with respect to the residual solvent peak. Coupling constants are reported in Hertz (Hz).

Thermogravimetric analyses (TGA) were carried out on a TG50 analyzer (Mettler-Toledo) and a SDT Q600 TG-DTA analyzer in air at a heating rate of 10 ºC min^{-1} within a temperature range of 40−600 °C.

Fourier transform infrared (FT-IR) spectra were recorded using a PerkinElmer FT-IR spectrometer equipped with an attenuated total reflectance (ATR) accessory. The spectra were background corrected and reported with a wave number (cm^{-1}) scale. The reflectance spectra were collected in the range of 4000-400 cm^{-1}.

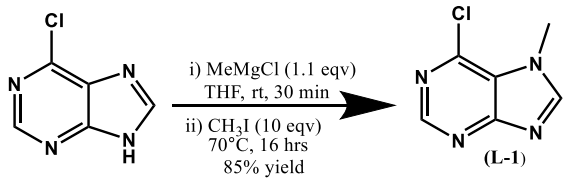
1.2 Crystal Structure refinement detail:

Single crystals of all nine MOFs were coated with light paraffin oil and mounted on a SuperNova, Dual, Cu at home/near Pilatus 200K diffractometer at 100K cooled with liquid nitrogen. Using Olexsys software[1], the structure was solved with the SHELXT[2] structure solution program using Intrinsic Phasing and refined with the SHELXL[3] refinement package using Least Squares minimization. Non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were fixed at calculated positions. The CCDC numbers of the crystals are **2344346-2344354.**

2 Chemical synthesis and characterization

All ligands, MCP, ACP, and BCP, were synthesized by following the reported procedure.[4]

2.1 Procedure for the synthesis of MCP (L-1):



To a 250 mL round bottom flask equipped with a magnetic stir bar, 2 g (12.94 mmol, 1 equiv.) of 6-chloro-9H-purine was added, and the flask was purged with N_2 several times after removal of air by high vacuum. 50 mL of THF was added to the RB, followed by 4.75 mL (14.234 mmol, 1.1 equiv.) of MeMgCl at 0°C. After 30 minutes, the ice bath was removed. Methyl Iodide (13 mL, 129.4 mmol, 10 equiv.) was added, and the reaction mixture was refluxed at 70°C for 16 hours. After this time, the TLC indicated the completion of the reaction. Methanol was added at room temperature to quench the reaction. The reaction mixture was evaporated under reduced pressure using a rotary evaporator, and the crude product was purified by column chromatography over silica gel (230-400 mesh) using 2% MeOH in DCM. 1.85 g of pure product was obtained (85% yield).^{1}H NMR (400 MHz, CD_3OD) δ (in ppm) = 8.75 (s, 1H), 8.59 (s, 1H), 4.18 (s, 3H); ^{13}C NMR (100 MHz, CD_3OD) δ (in ppm) = 162.44, 152.98, 152.28, 145.01, 124.5, 34.82

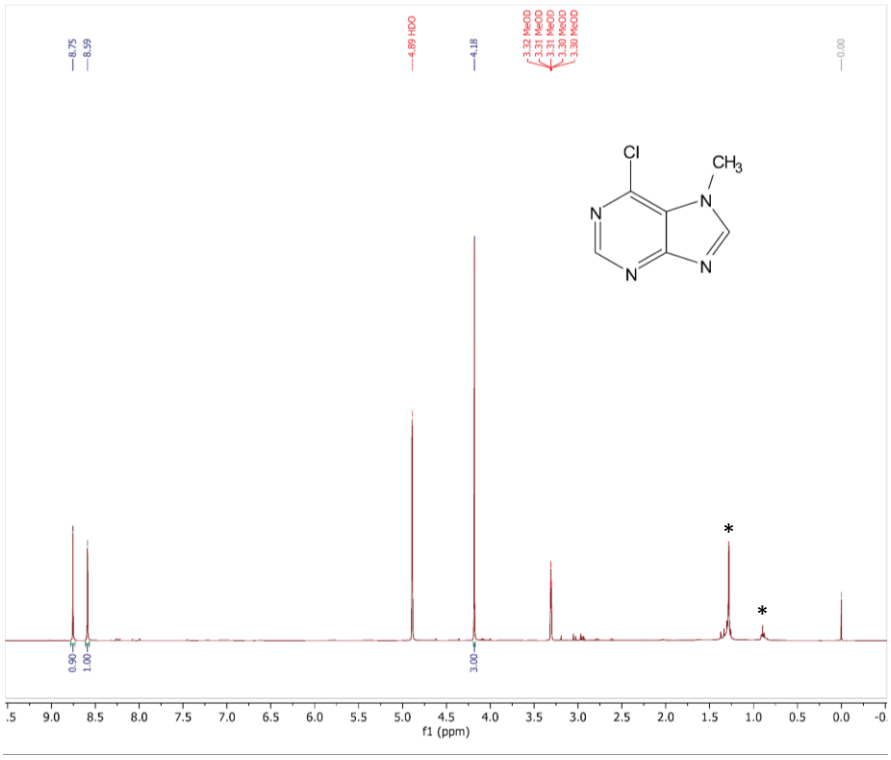


Figure S1. ^{1}H NMR spectrum (400 MHz, 298K, CD_3OD) of MCP (**L1)** (* is the grease peak)[5]

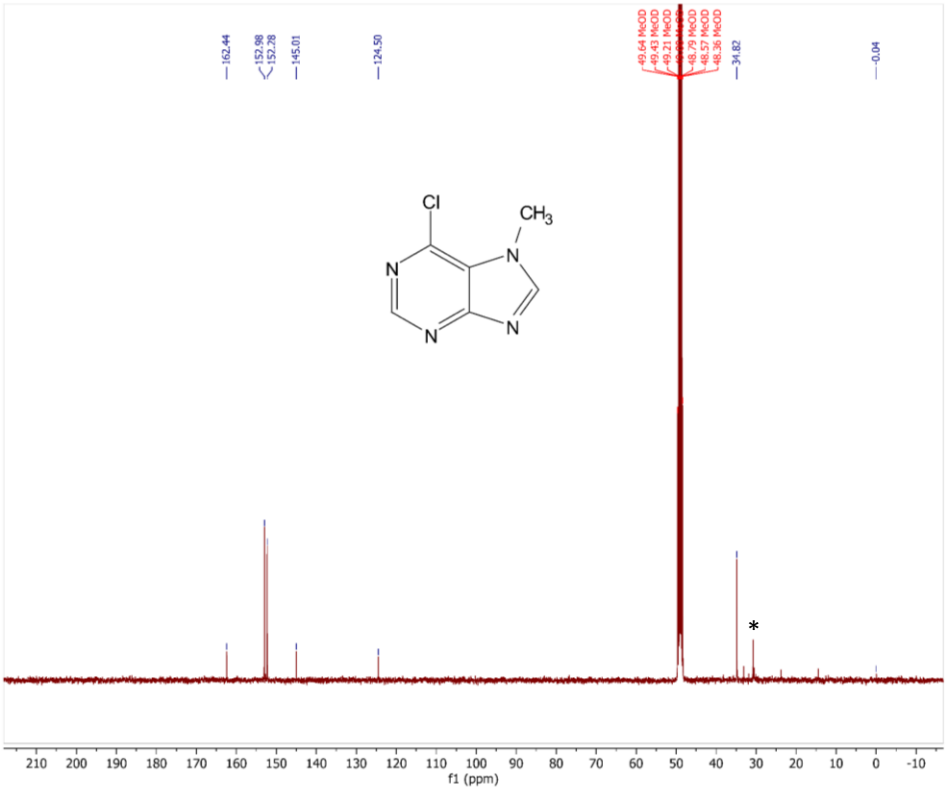
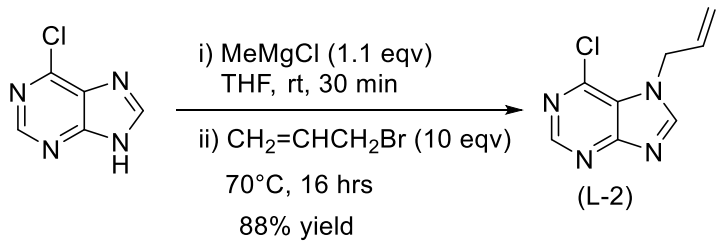


Figure S2. ^{13}C NMR spectrum (100 MHz, 298K, CD_3OD) of MCP (**L1)** (* is the grease peak)[5]

2.2 Procedure for the synthesis of ACP (L-2):



To a 250 mL round bottom flask equipped with a magnetic stir bar, 2g (12.94 mmol, 1 equiv.) of 6-chloro-9H-purine was added, and the flask was purged with N_2 several times after removal of air by high vacuum. Later, 50 mL of THF was added to the RB, followed by the 4.75mL (14.234 mmol, 1.1 equiv.) of MeMgCl at 0°C. The reaction mixture was stirred at room temperature for 30 minutes. The allyl bromide 11.2 mL (129.4 mmol, 10 equiv.) was added, and the reaction was refluxed at 70°C for 16 hours. After this time, TLC indicated the completion of the reaction; methanol was added to quench the reaction at room temperature. The reaction mixture was evaporated under reduced pressure, and the crude reaction mixture was purified by column chromatography over silica gel (230-400 mesh) by 2% (MeOH/DCM). The pure product obtained was 2.2g (88% yield). ^{1}H NMR (400 MHz, CD_3OD) δ (in ppm) = 8.79 (s, 1H), 8.69 (s,1H), 6.18 (m, 1H), 5.32 (d, 1H), 5.21 (m, 2H), 5.05(d, 1H); ^{13}C NMR (101 MHz, CD_3OD) δ (in ppm) = 161.2, 151.77, 150.44, 143.36, 132.98, 122.42, 117.28, 48.83

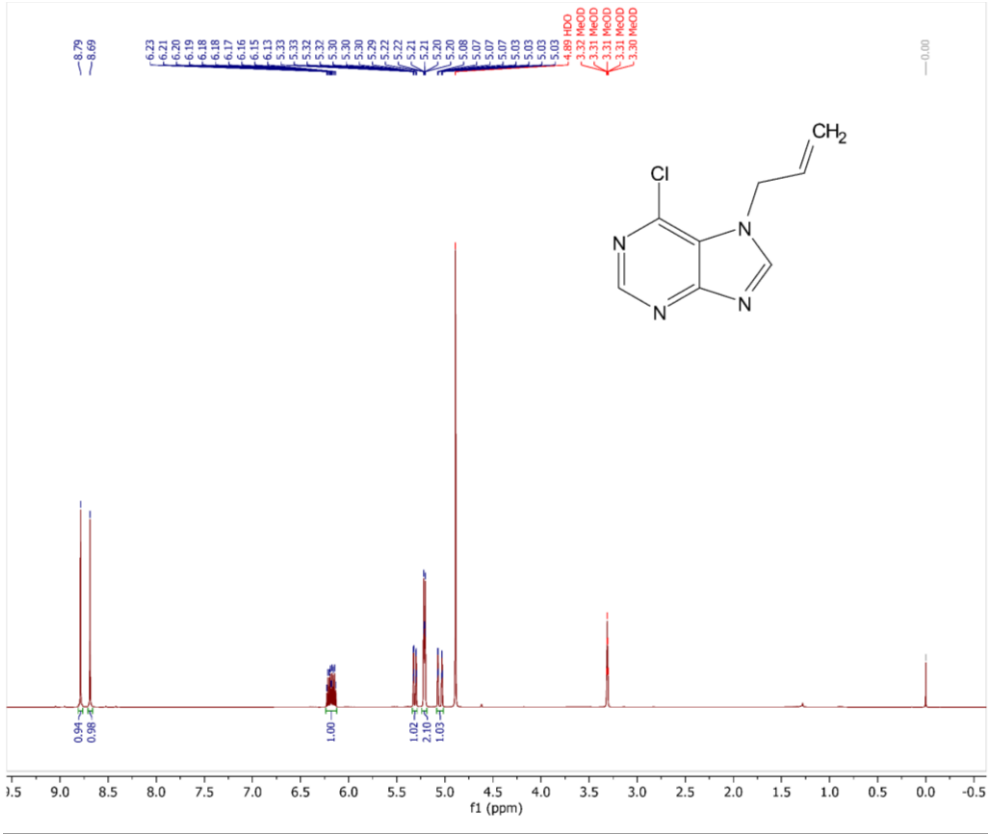


Figure S3. ^{1}H NMR spectrum (400 MHz, 298K, CD_3OD) of ACP (**L-2)**.

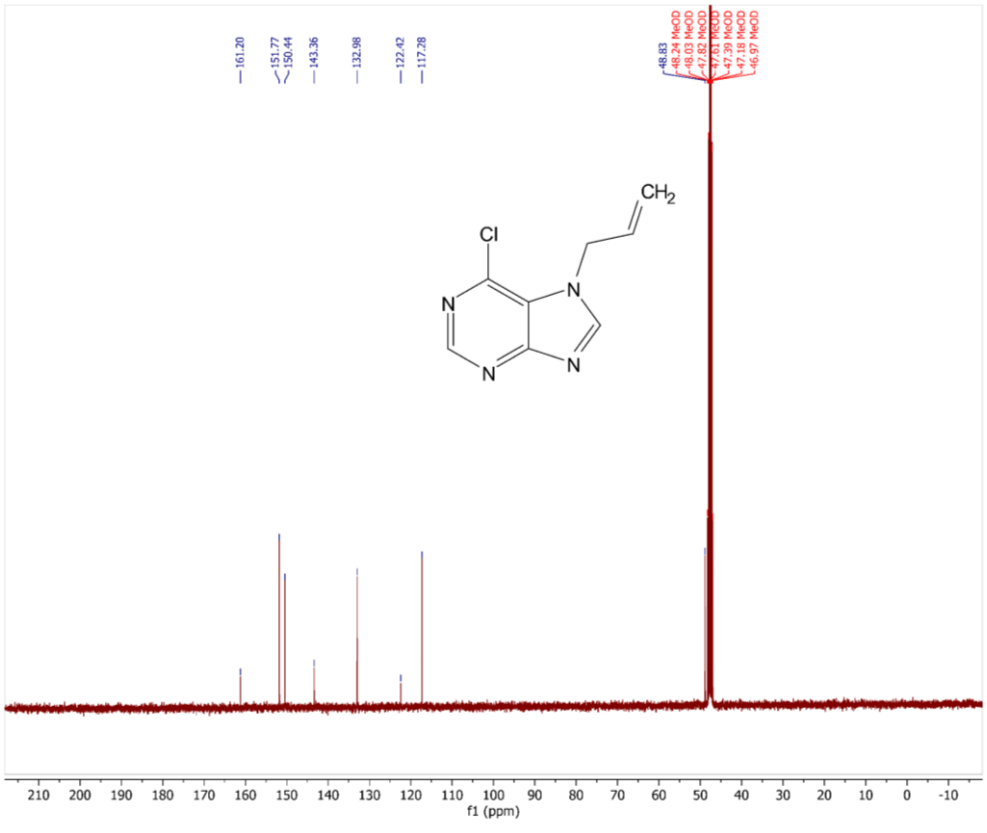
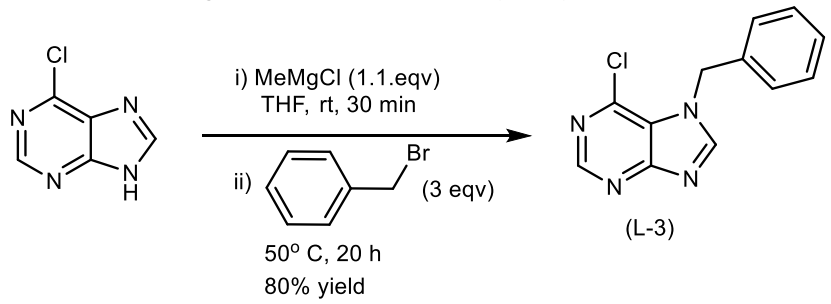


Figure S4. ^{13}C NMR spectrum (100 MHz, 298K, CD_3OD) of ACP (**L-2)**.

2.3 Procedure for the synthesis of BCP (L-3):



To a 250 mL round bottom flask equipped with a magnetic stir bar, 3g (19.40 mmol, 1 equiv.) of 6-chloro-9H-purine was added, and the flask was purged with N_2 several times after removal of air by high vacuum. Later, 50 mL of THF was added to the RB, followed by the 7.10mL (21.34 mmol, 1.1 equiv.) of MeMgCl at 0°C. The reaction mixture was stirred at room temperature for 30 minutes. The benzyl bromide 6.9mL (58.2 mmol, 3 equiv.) was added, and the reaction was refluxed at 50°C for 20 hours. After this time, TLC indicated the completion of the reaction; methanol was added to quench the reaction at room temperature. The reaction mixture was evaporated under reduced pressure, and the crude reaction mixture was purified by column chromatography over silica gel (230-400 mesh) by 1% (MeOH/DCM). The pure product obtained was 3.80g (80% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.90 (s, 1H), 8.22 (s, 1H), 7.39 (h, J = 3.6 Hz, 3H), 7.18 (dd, J = 7.2, 2.4 Hz, 2H), 5.69 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.14, 152.74, 149.25, 143.35, 134.72, 129.51, 129.05, 127.19, 122.67, 77.48, 77.16, 76.84, 50.86.

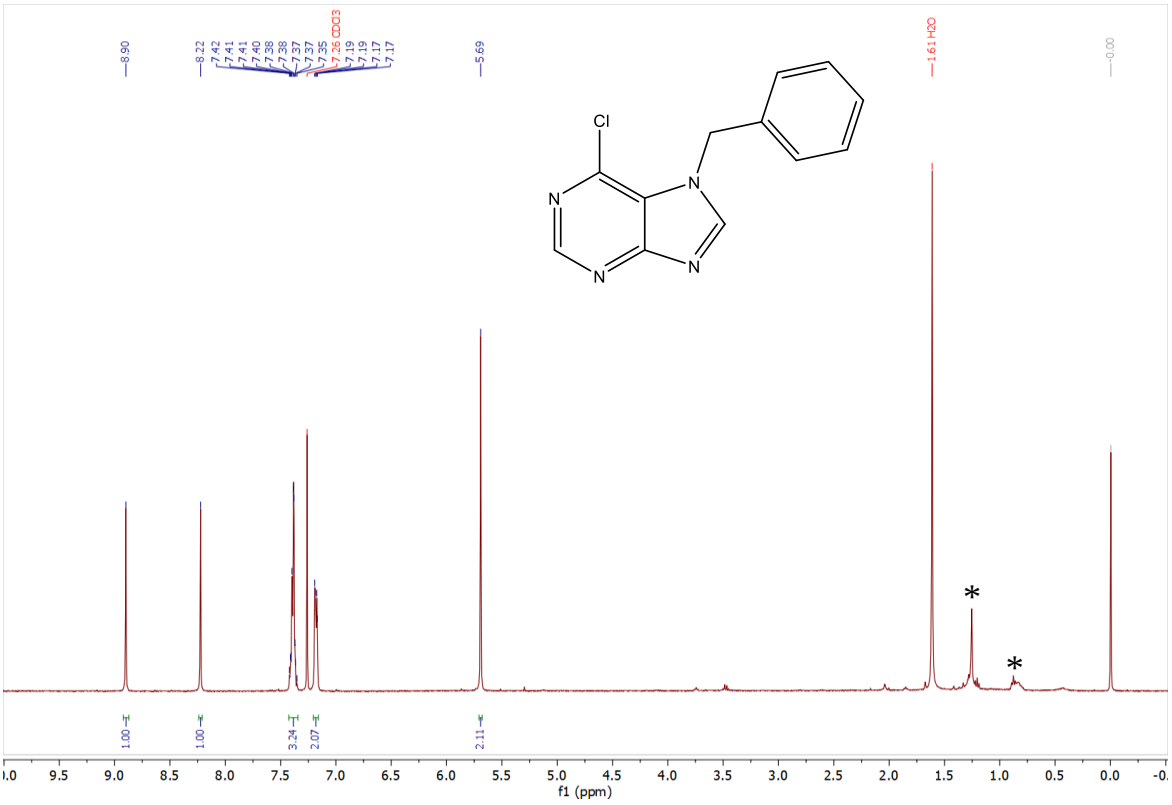


Figure S5. ^{1}H NMR spectrum (400 MHz, 298K, $CDCl_3$) of BCP (**L-3)** (* is the grease peak).

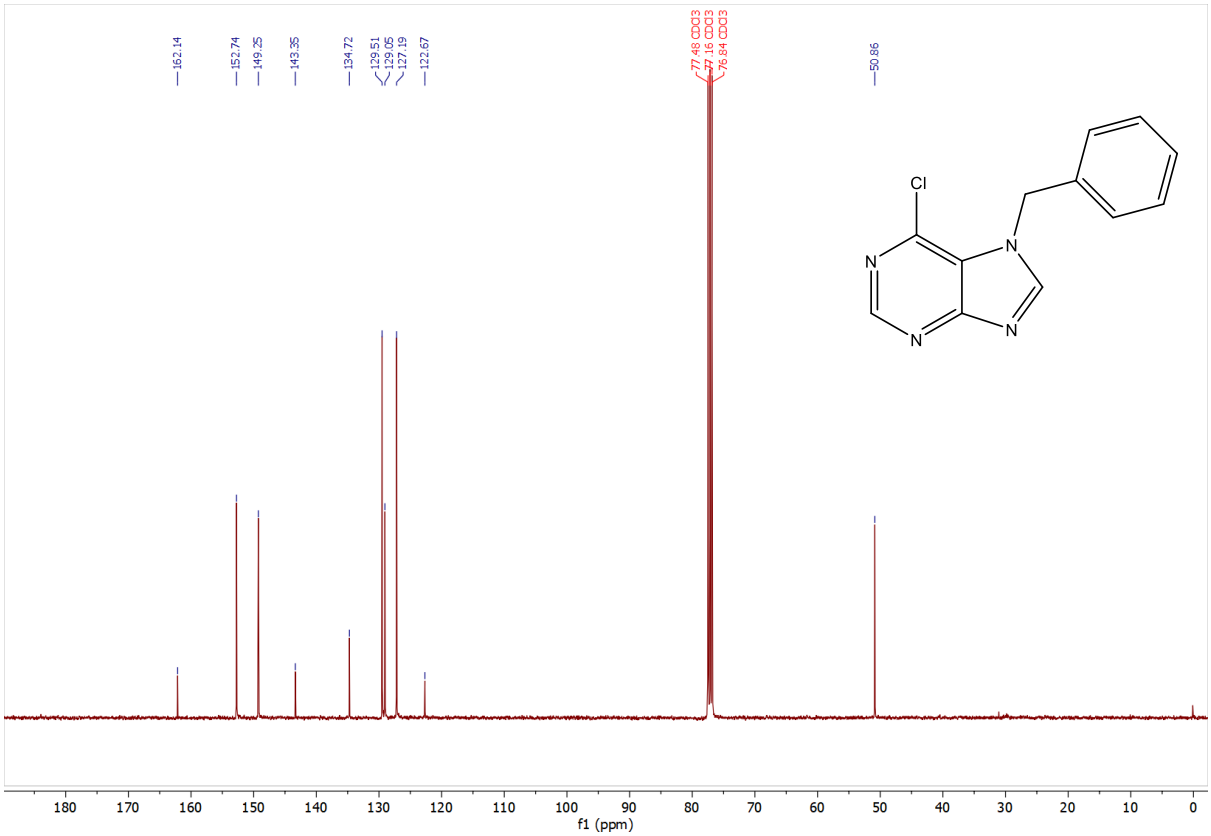


Figure S6. ^{13}C NMR spectrum (100 MHz, 298K, $CDCl_3$) of BCP (**L-3)**.

3 Powder Xrd diffraction:

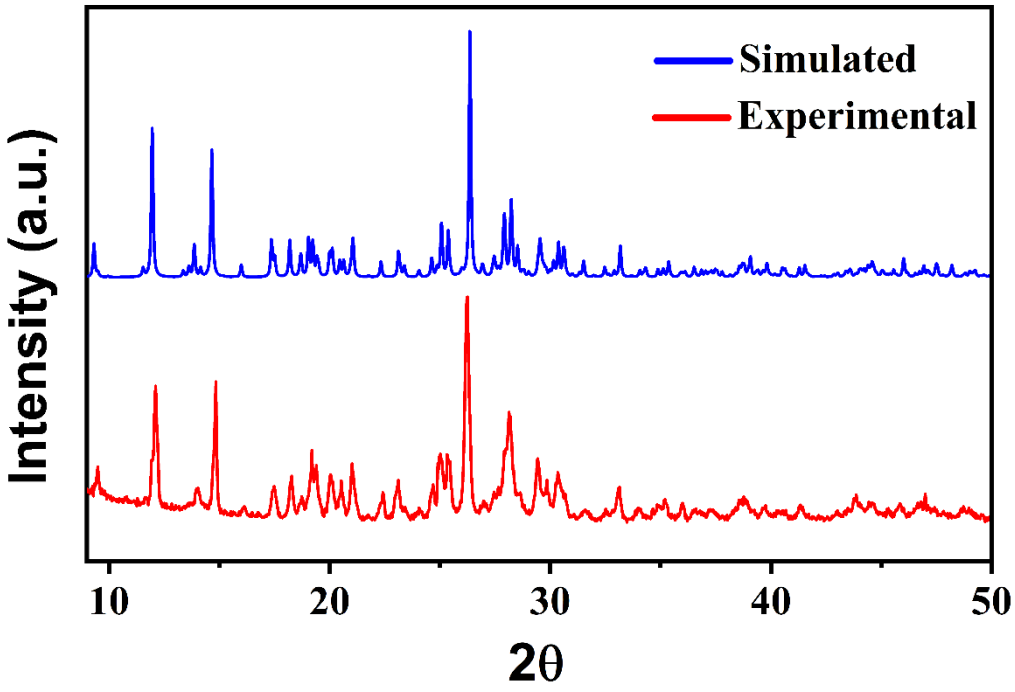


Figure S7. Simulated (upper, blue) and experimental (lower, red) X-ray powder diffraction patterns of ZnMCP.

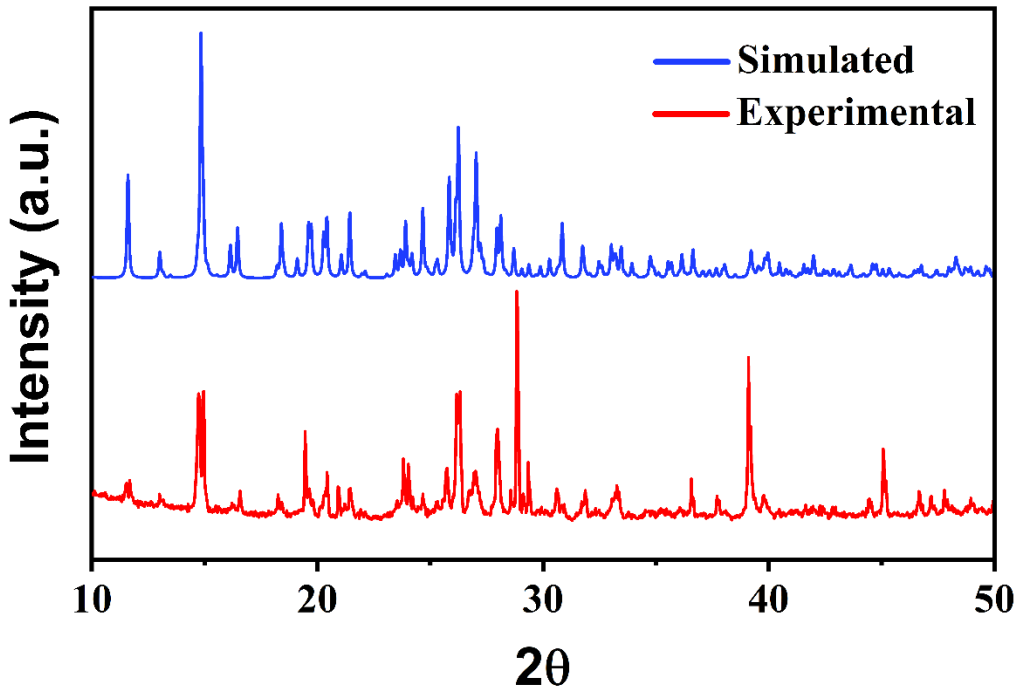


Figure S8. Simulated (upper, blue) and experimental (lower, red) X-ray powder diffraction patterns of ZnACP.

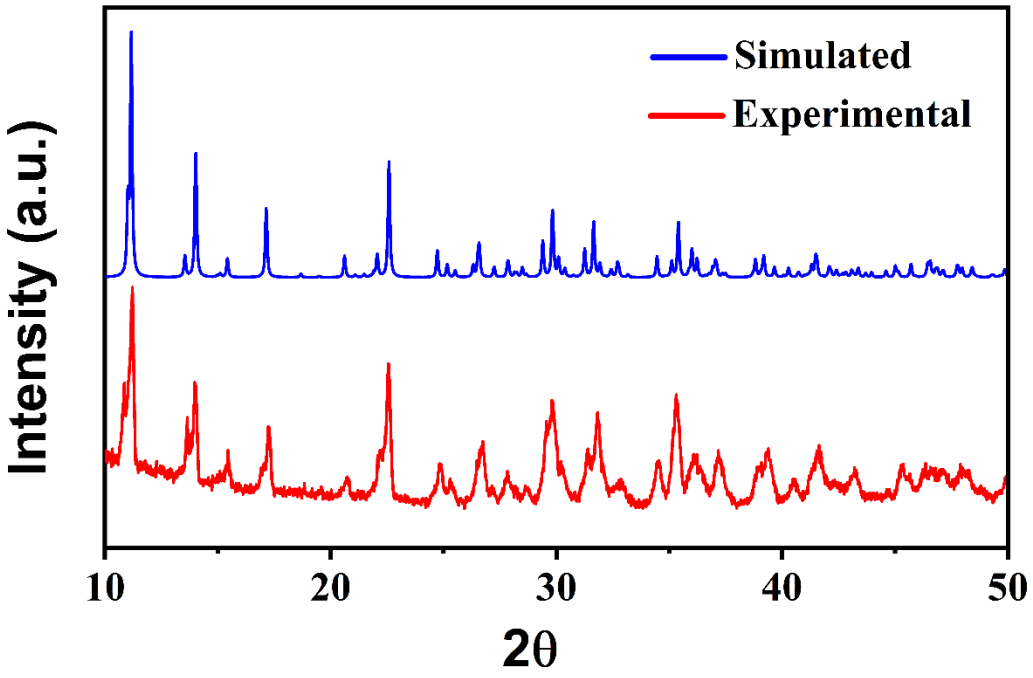


Figure S9. Simulated (upper, blue) and experimental (lower, red) X-ray powder diffraction patterns of CdMCP.

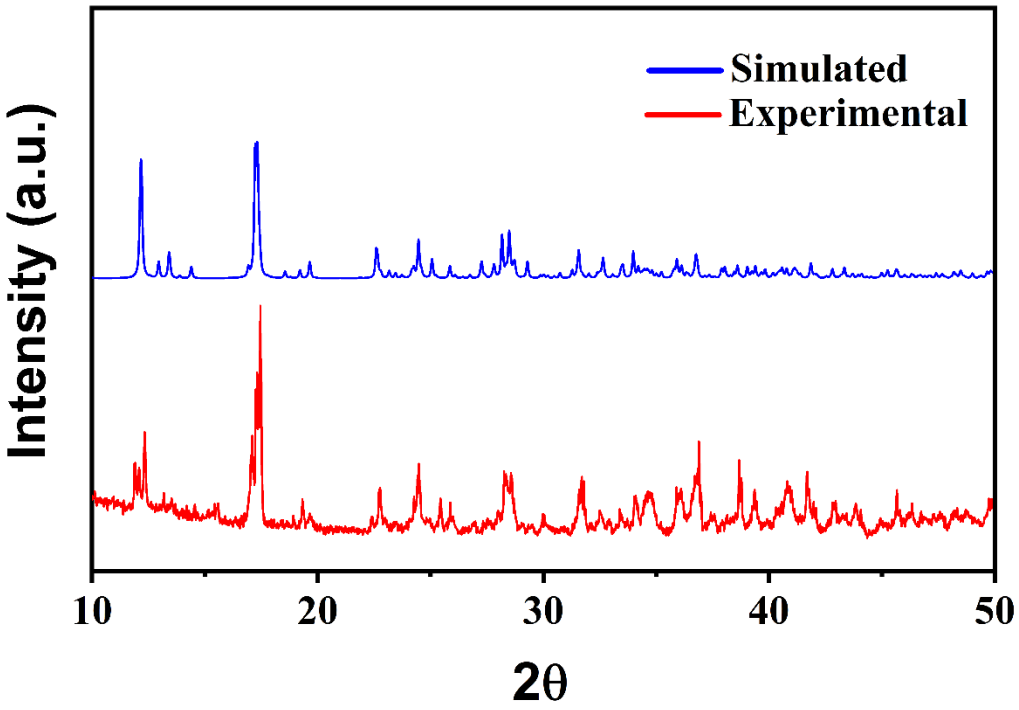


Figure S10. Simulated (upper, blue) and experimental (lower, red) X-ray powder diffraction patterns of CdACP.

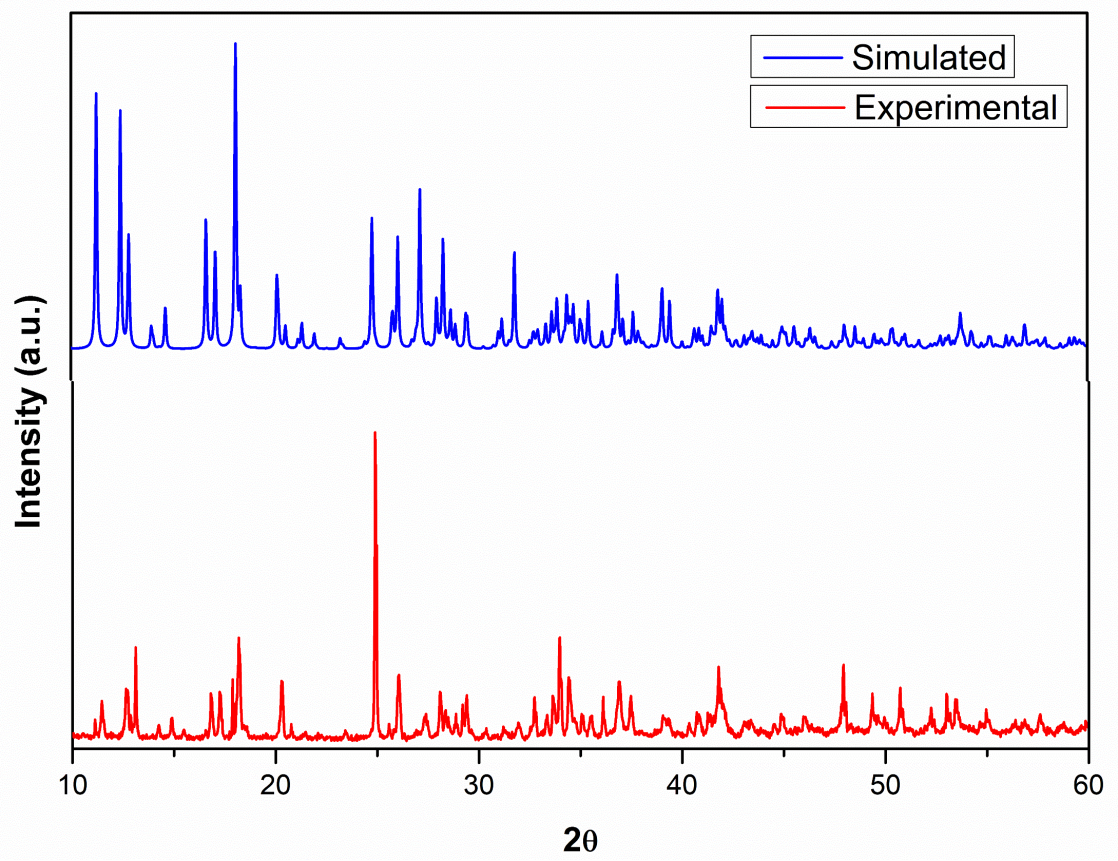


Figure S11. Simulated (upper, blue) and experimental (lower, red) X-ray powder diffraction patterns of CdBCP.

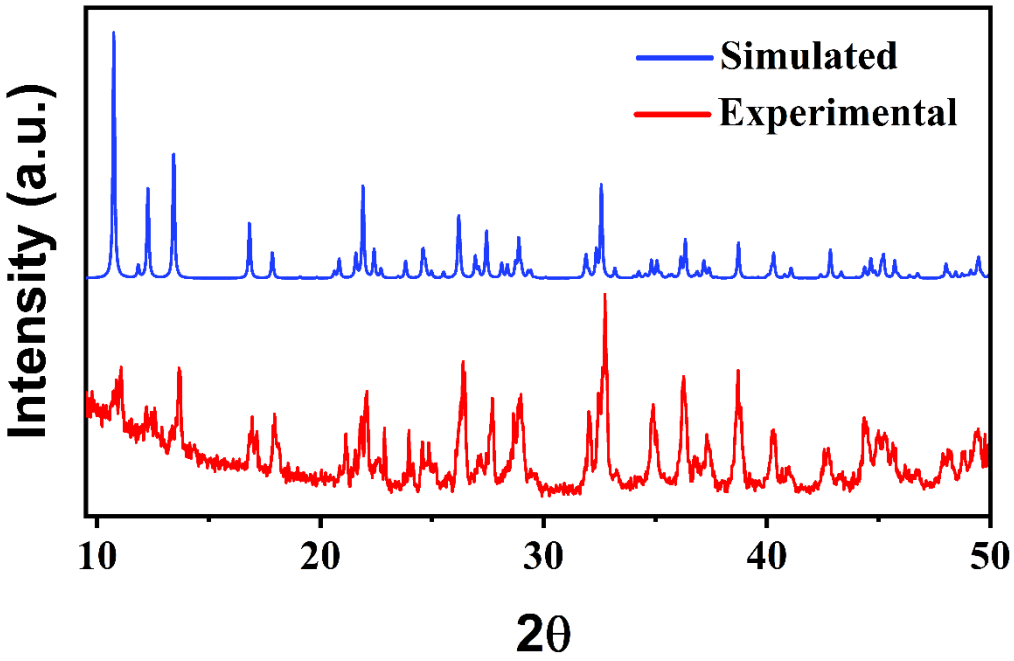


Figure S12. Simulated (upper, blue) and experimental (lower, red) X-ray powder diffraction patterns of HgMCP.

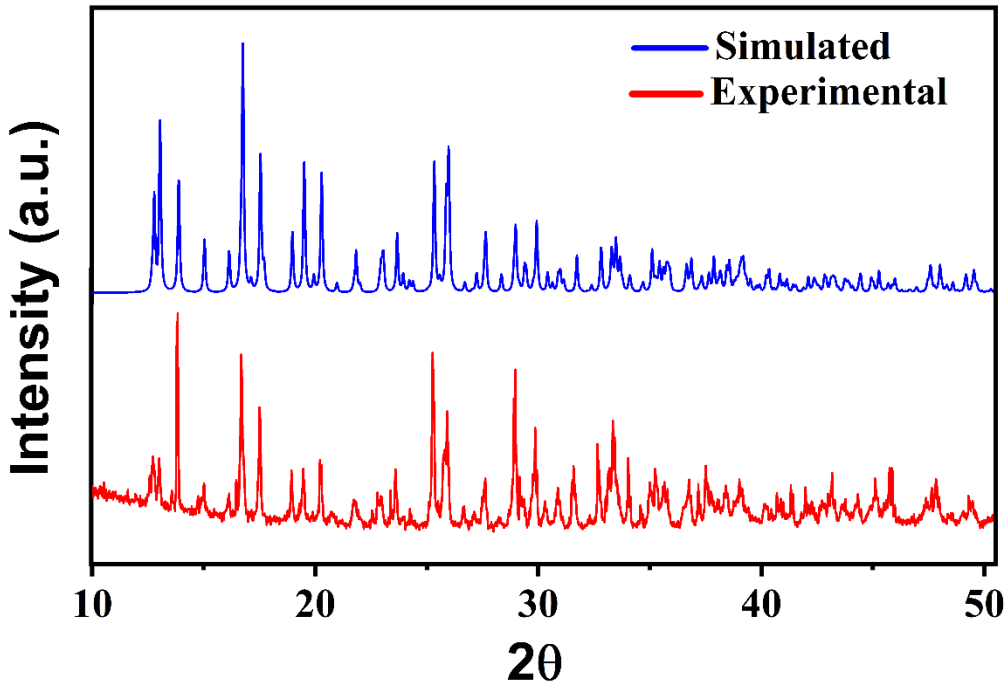


Figure S13. Simulated (upper, blue) and experimental (lower, red) X-ray powder diffraction patterns of HgBCP.

4 ORTEP diagram:

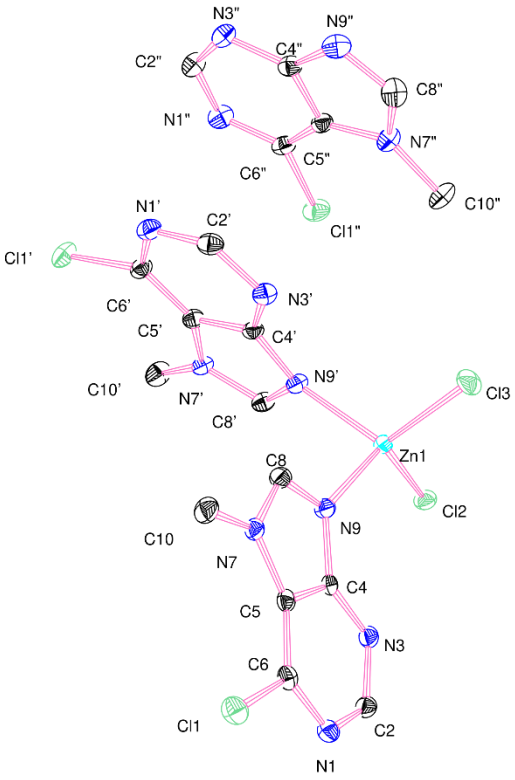


Figure S14. ORTEP diagram of ZnMCP (50% probability).

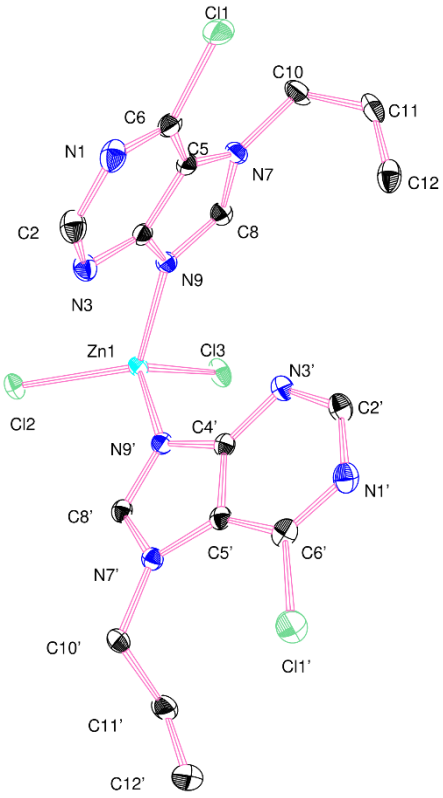


Figure S15. ORTEP diagram of ZnACP (50% probability).

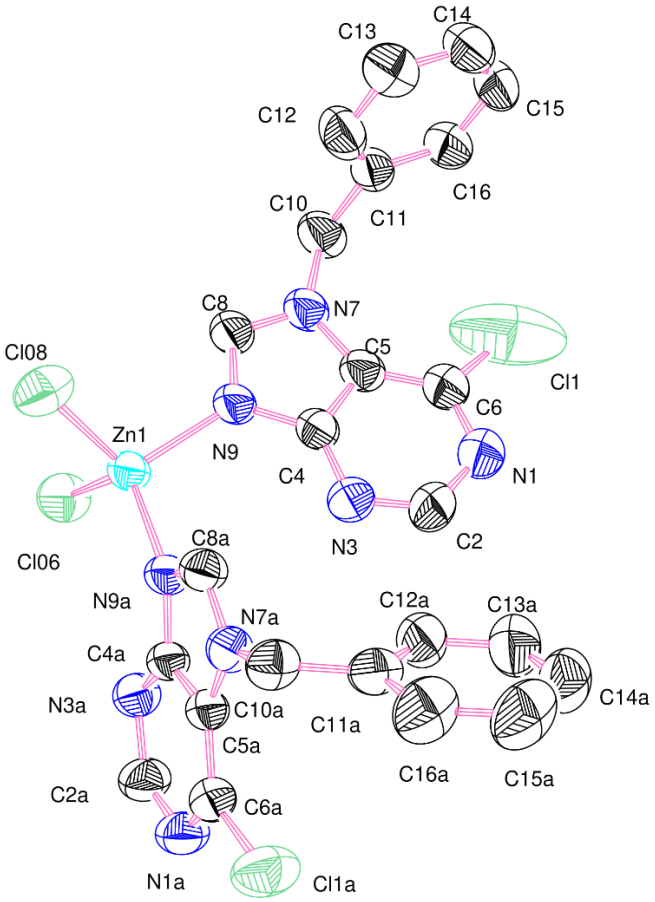


Figure S16. ORTEP diagram of ZnBCP (50% probability).

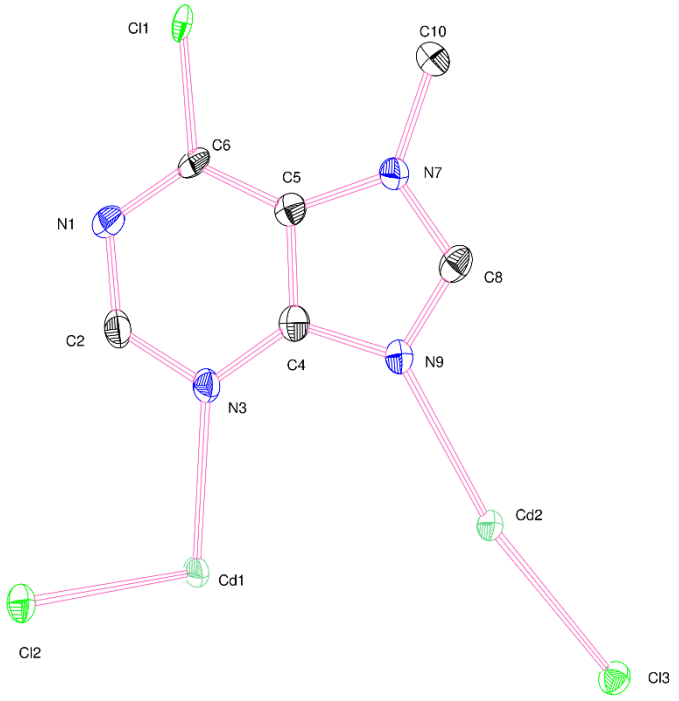


Figure S17. ORTEP diagram of CdMCP (50% probability).

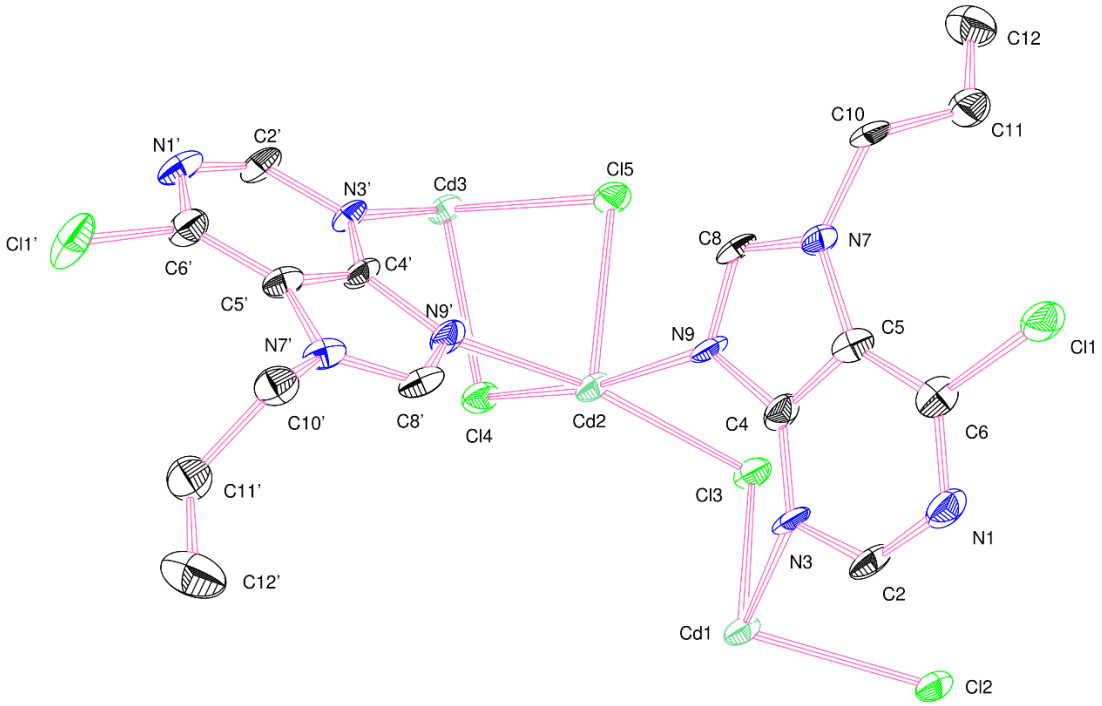


Figure S18. ORTEP diagram of CdACP (50% probability).

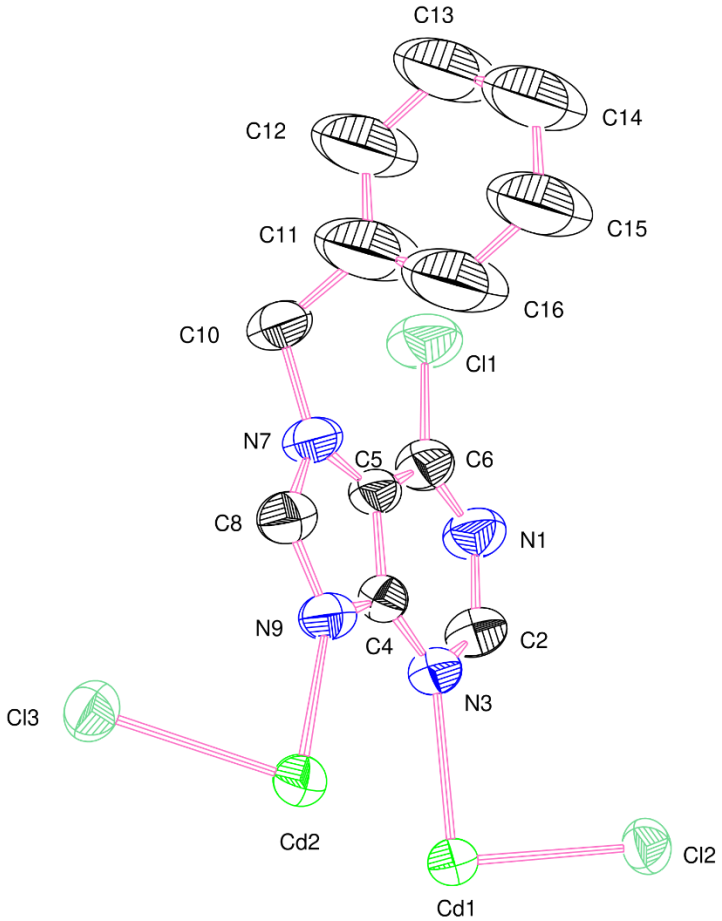


Figure S19. ORTEP diagram of CdBCP (50% probability).

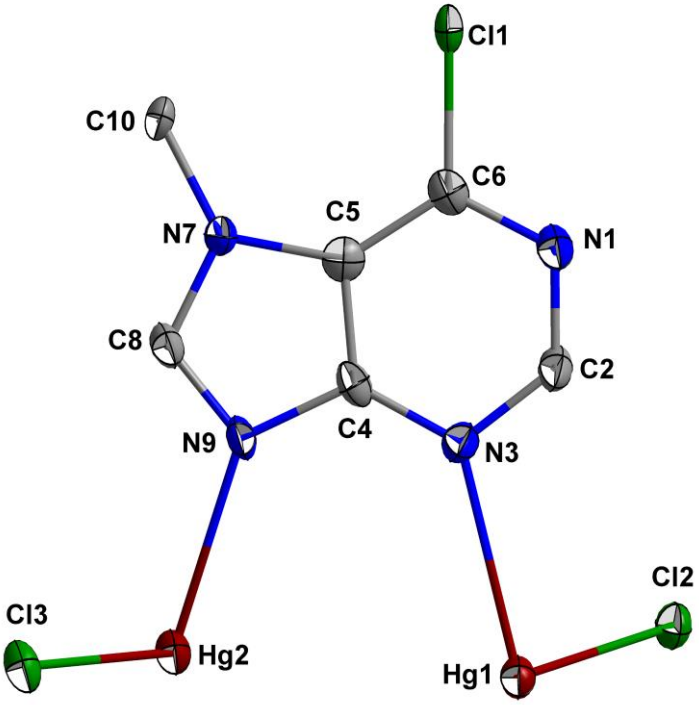


Figure S20. ORTEP diagram of HgMCP (50% probability).

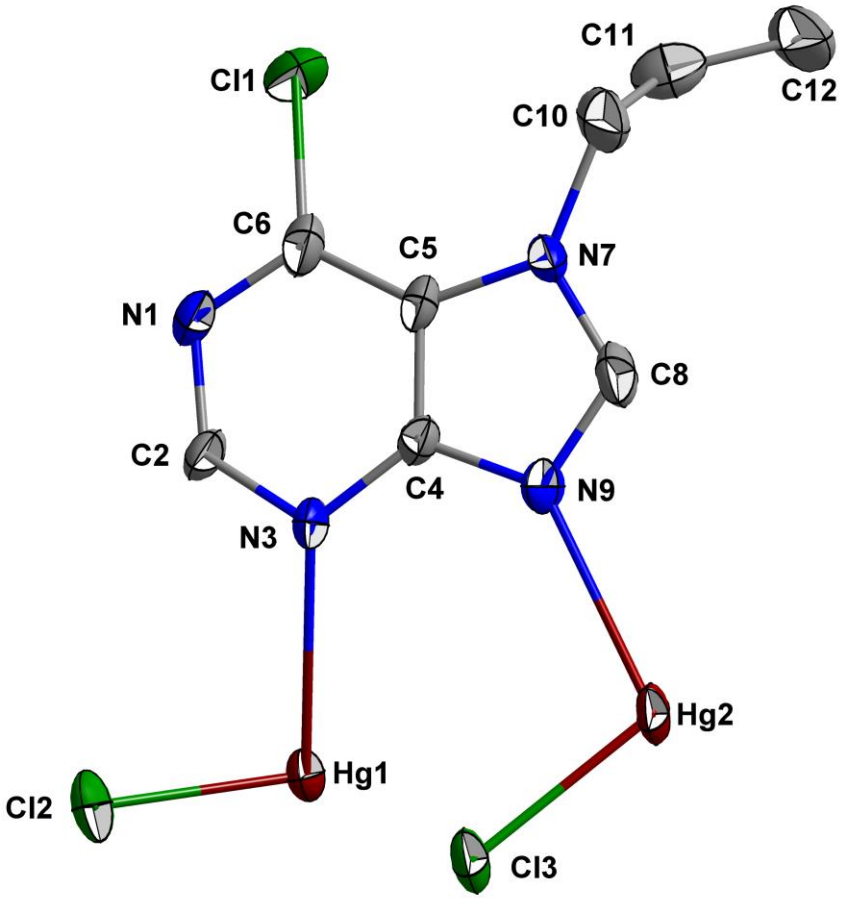


Figure S21. ORTEP diagram of HgACP (50% probability).

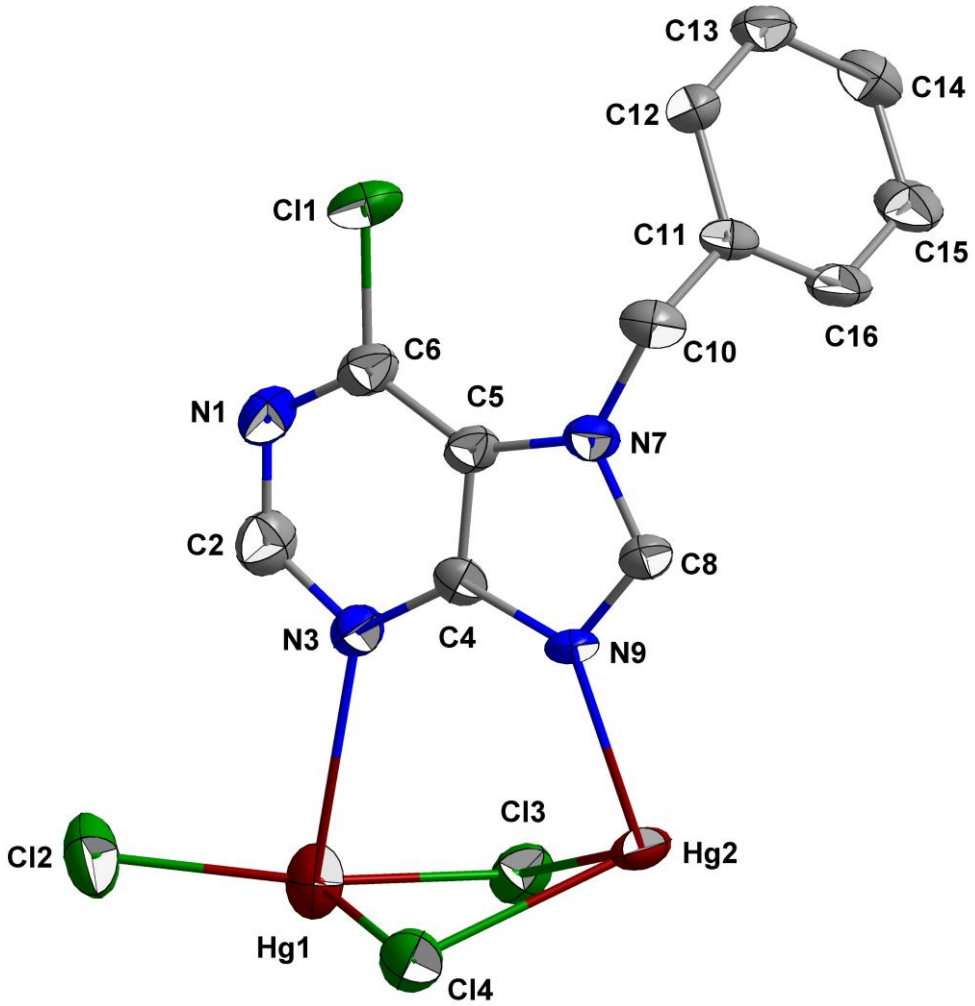


Figure S22. ORTEP diagram of HgBCP (50% probability). [Bond length of Hg1-N3 is 2.749 Å, but due to some technical problem in ortep3 (v1.0.3), the bond is not showing.]

5 ^{1}H NMR spectra of Zn and Hg MOFS:

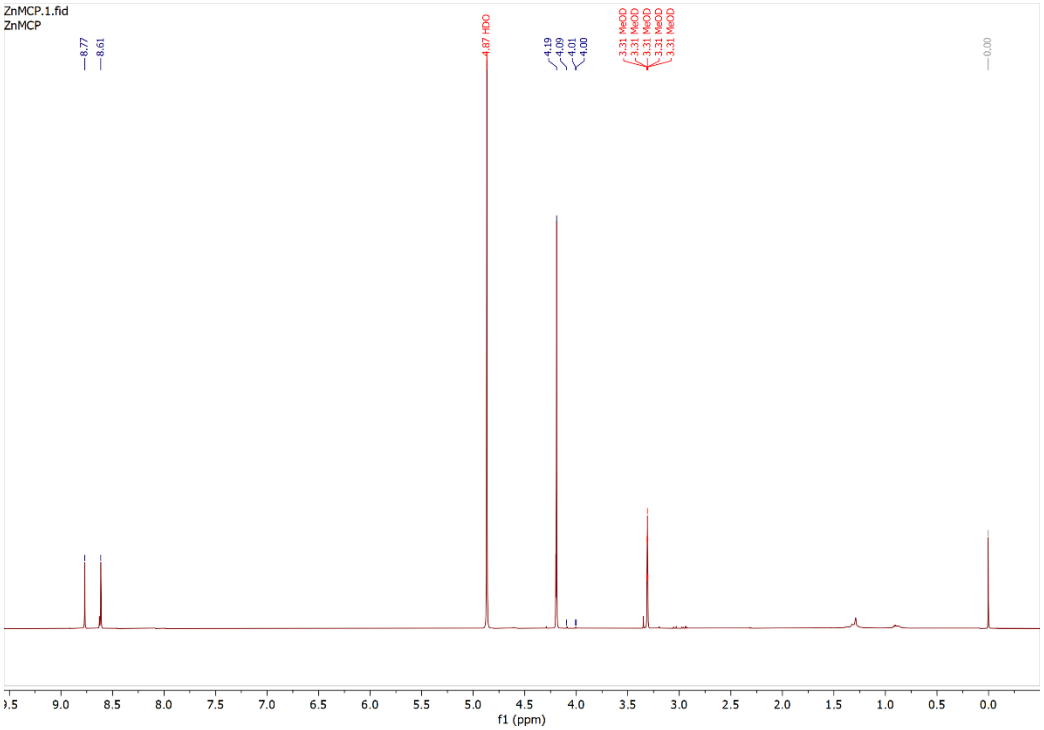


Figure S23. ^{1}H NMR spectrum (700 MHz, 298K, CD_3OD) of ZnMCP.

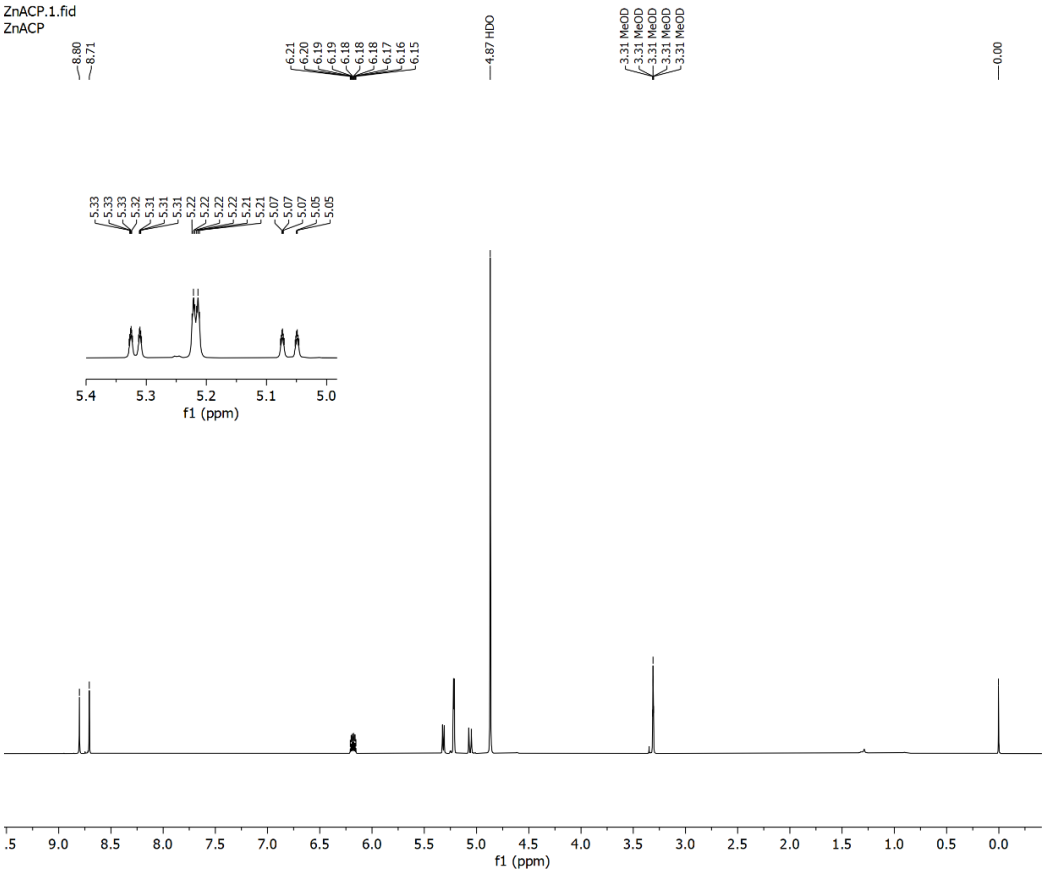


Figure S24. ^{1}H NMR spectrum (700 MHz, 298K, CD_3OD) of ZnACP.

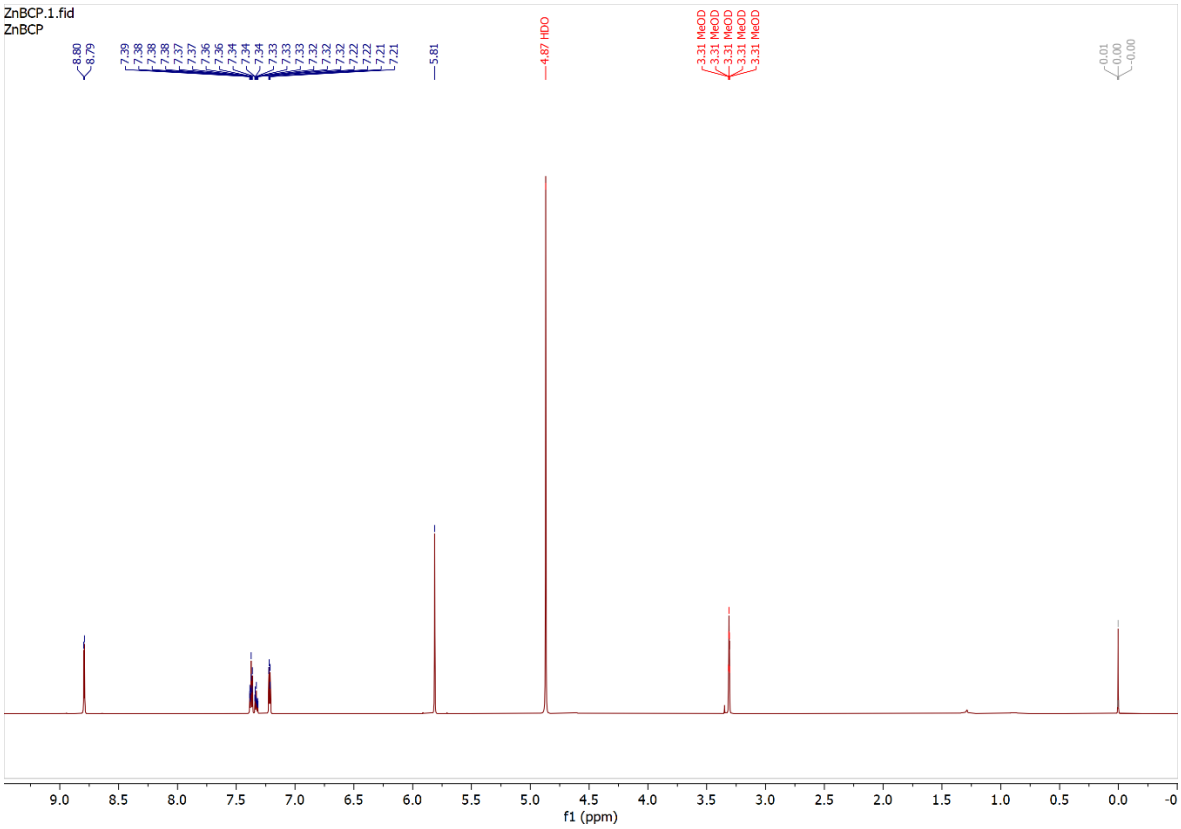


Figure S25. ^{1}H NMR spectrum (700 MHz, 298K, CD_3OD) of ZnBCP.

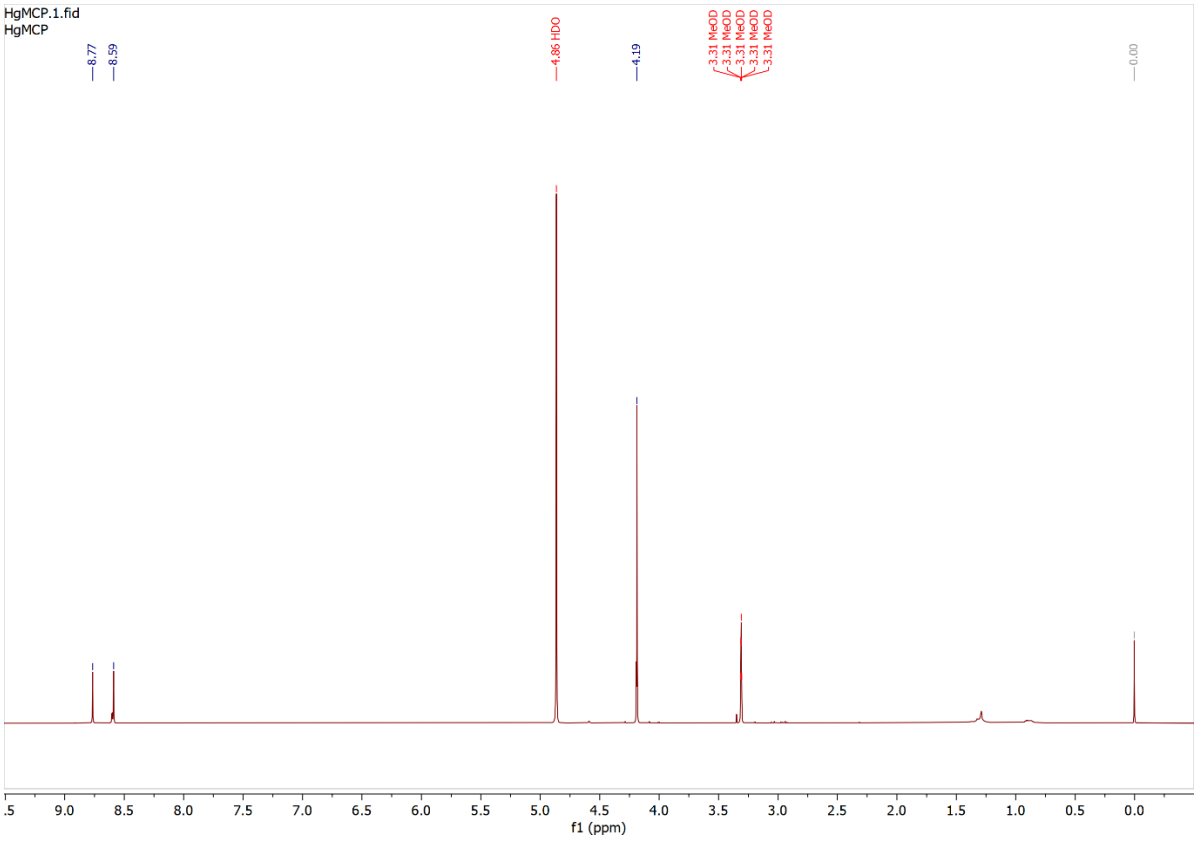


Figure S26. ^{1}H NMR spectrum (700 MHz, 298K, CD_3OD) of HgMCP.

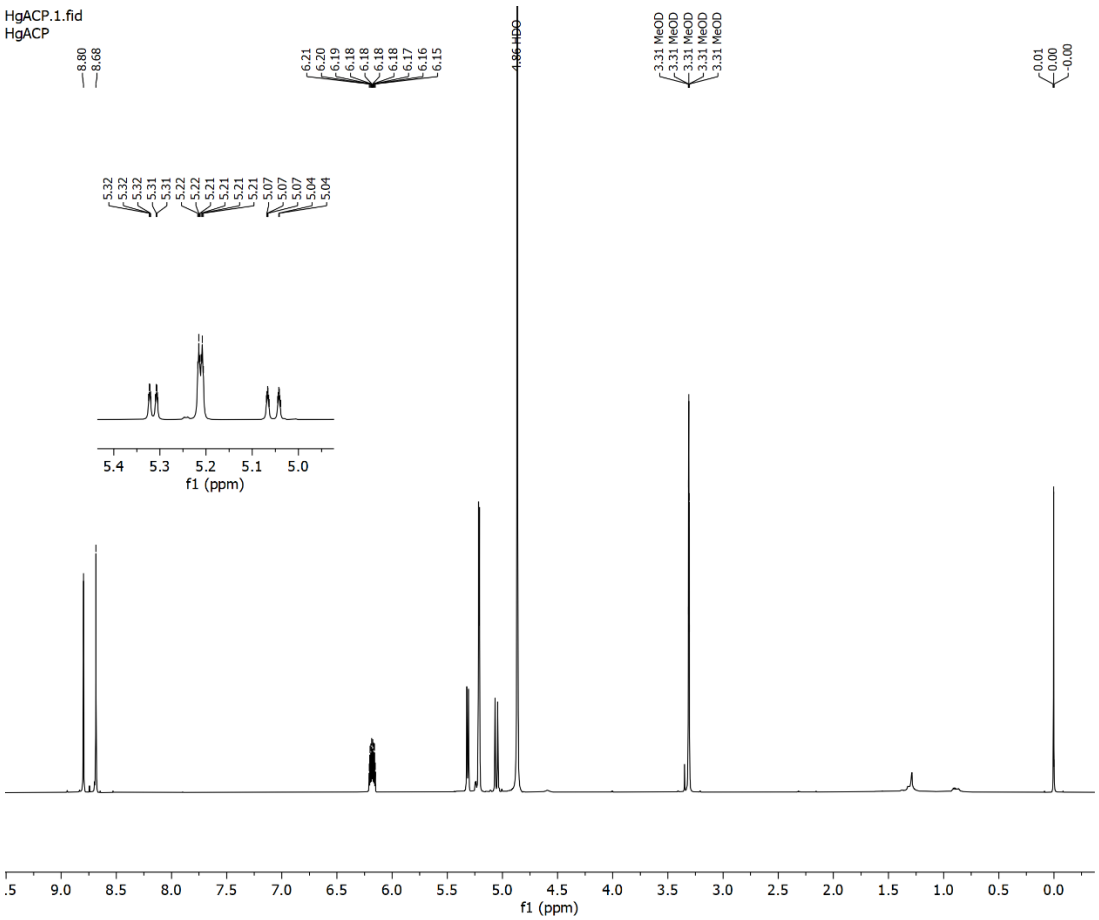


Figure S27. ^{1}H NMR spectrum (700 MHz, 298K, CD_3OD) of HgACP.

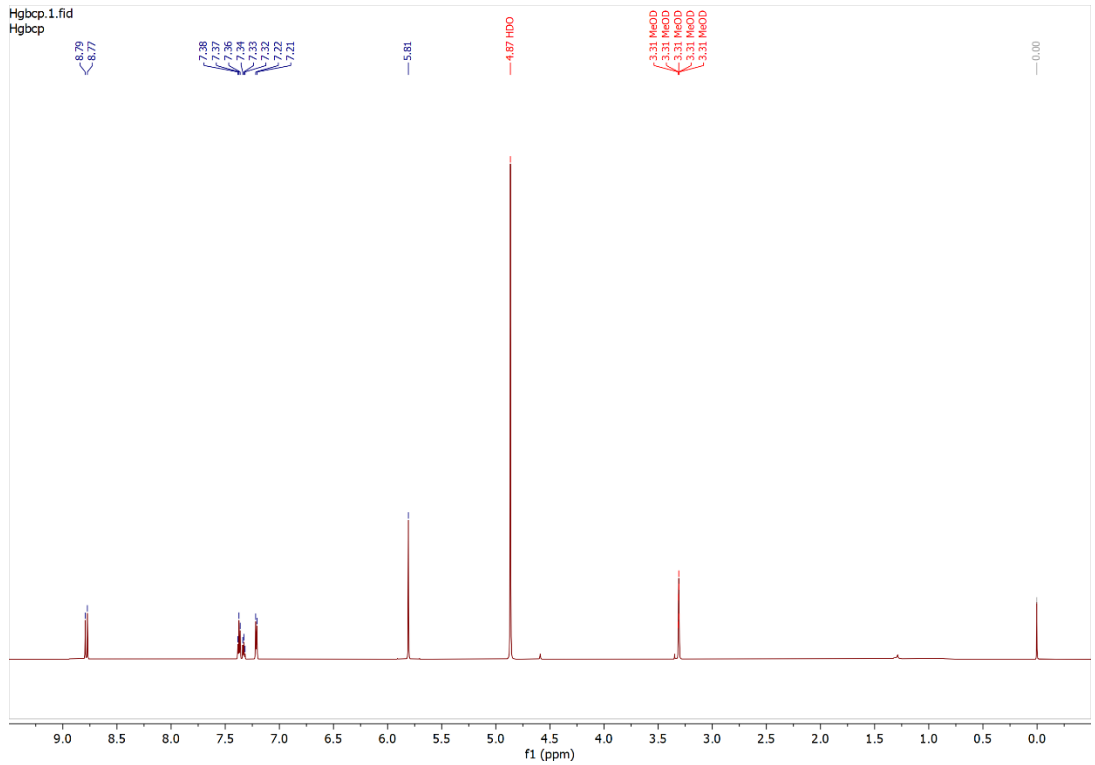


Figure S28. ^{1}H NMR spectrum (700 MHz, 298K, CD_3OD) of HgBCP.

6 Thermogravimetric Analysis

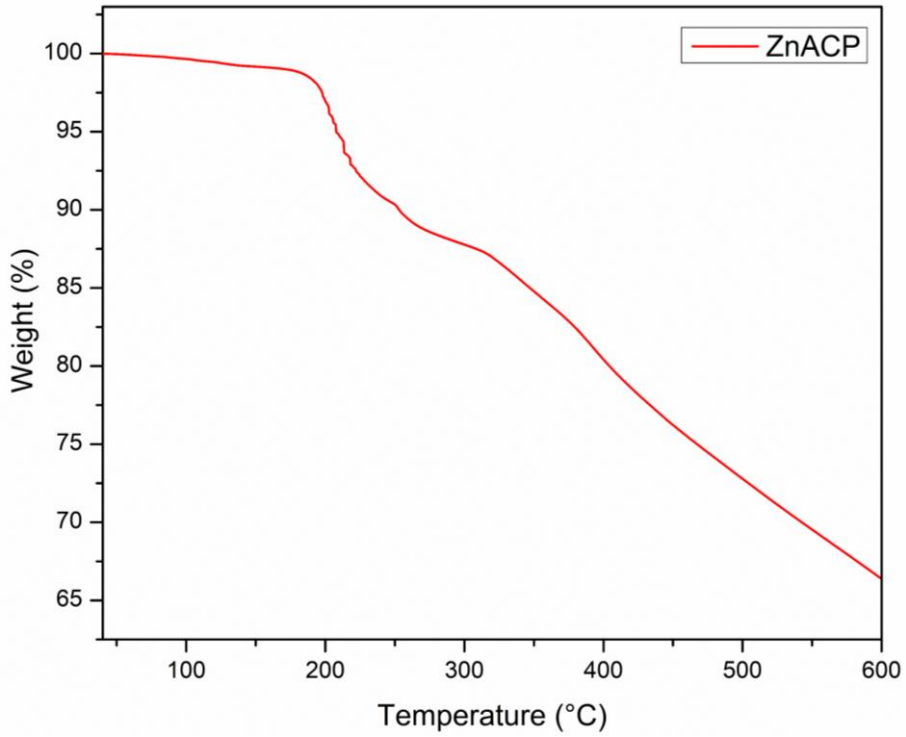


Figure S29. TGA of ZnACP.

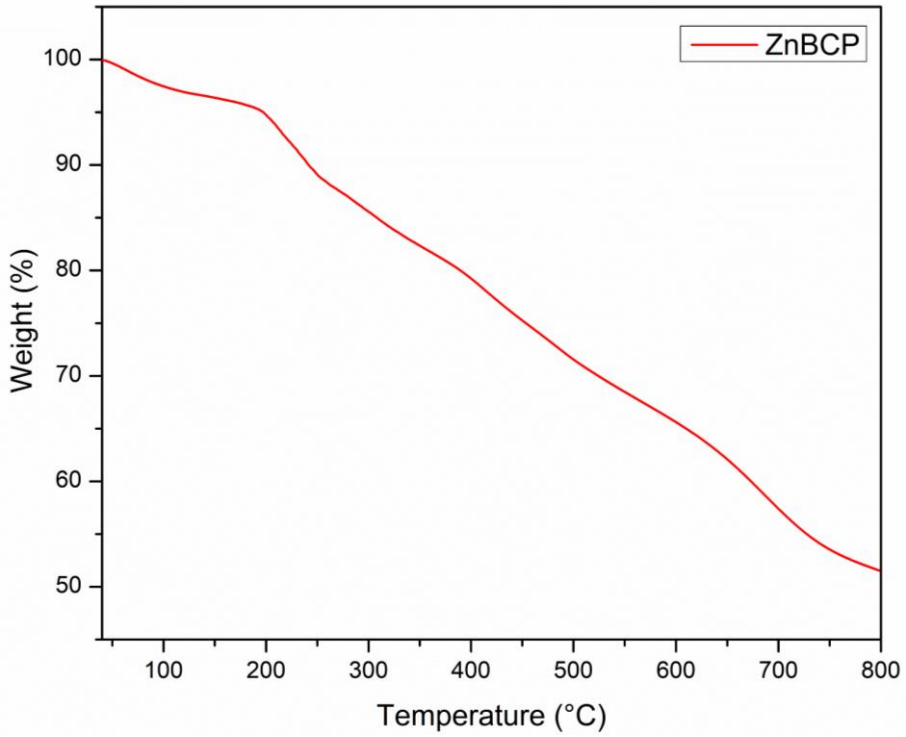


Figure S30. TGA of ZnBCP.

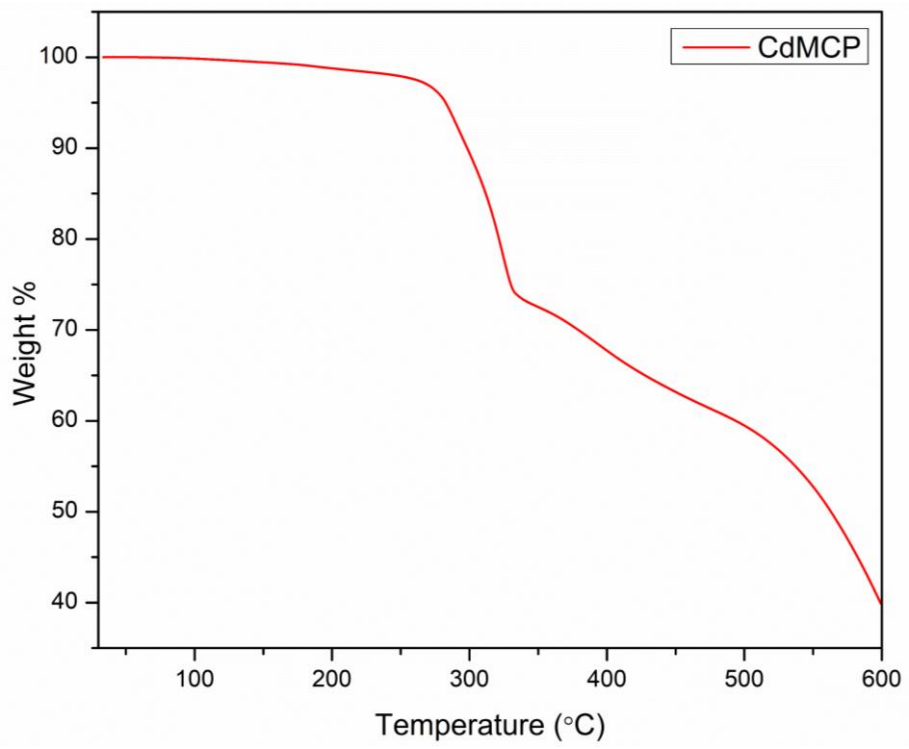


Figure S31. TGA of CdMCP.

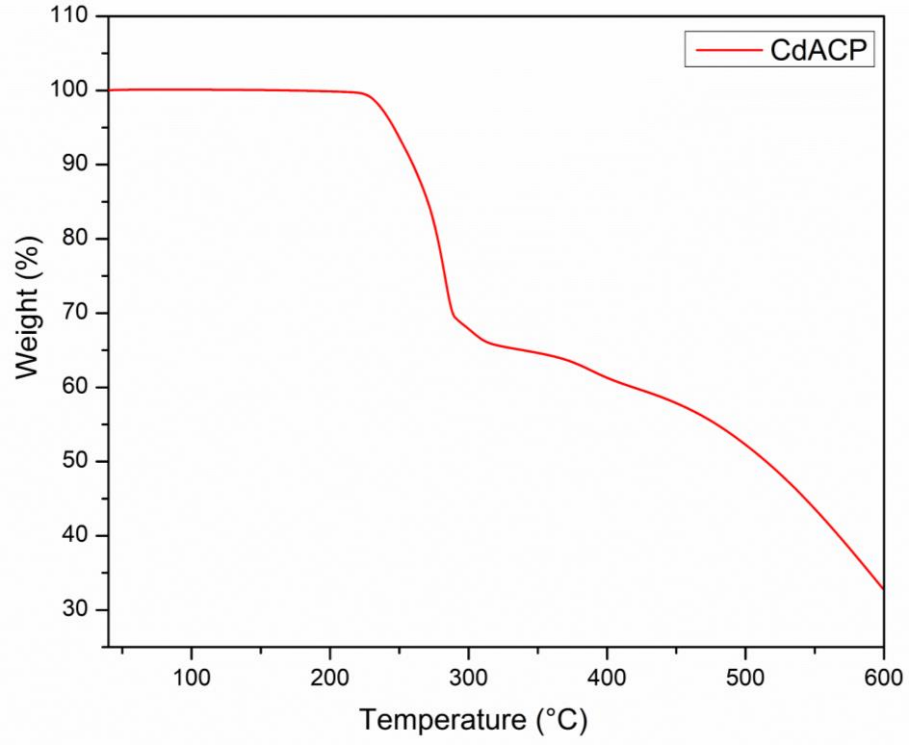


Figure S32. TGA of CdACP.

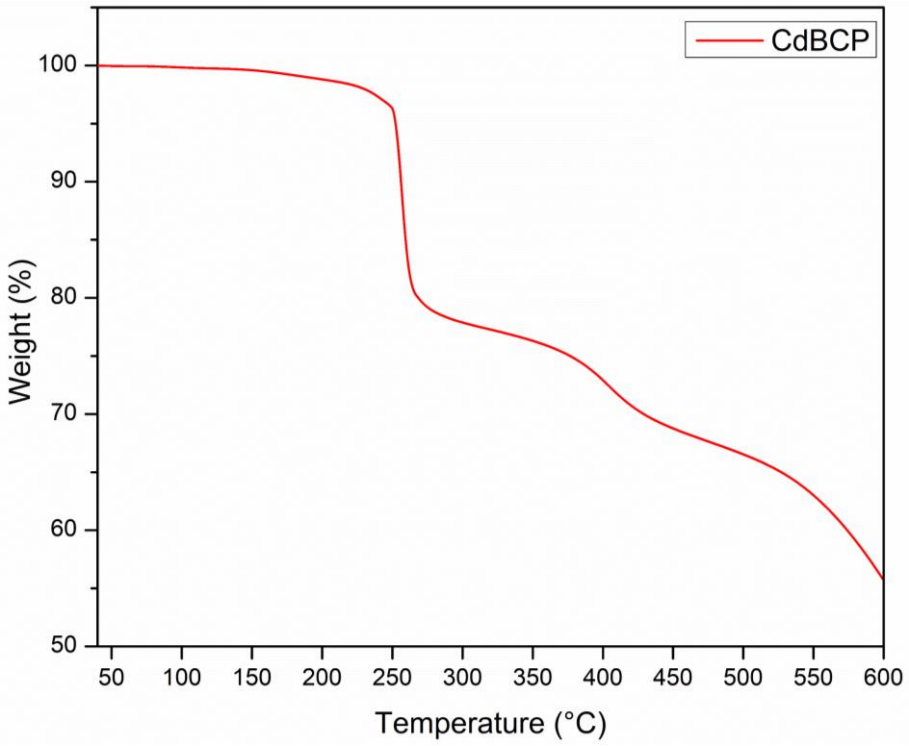


Figure S33. TGA of CdBCP.

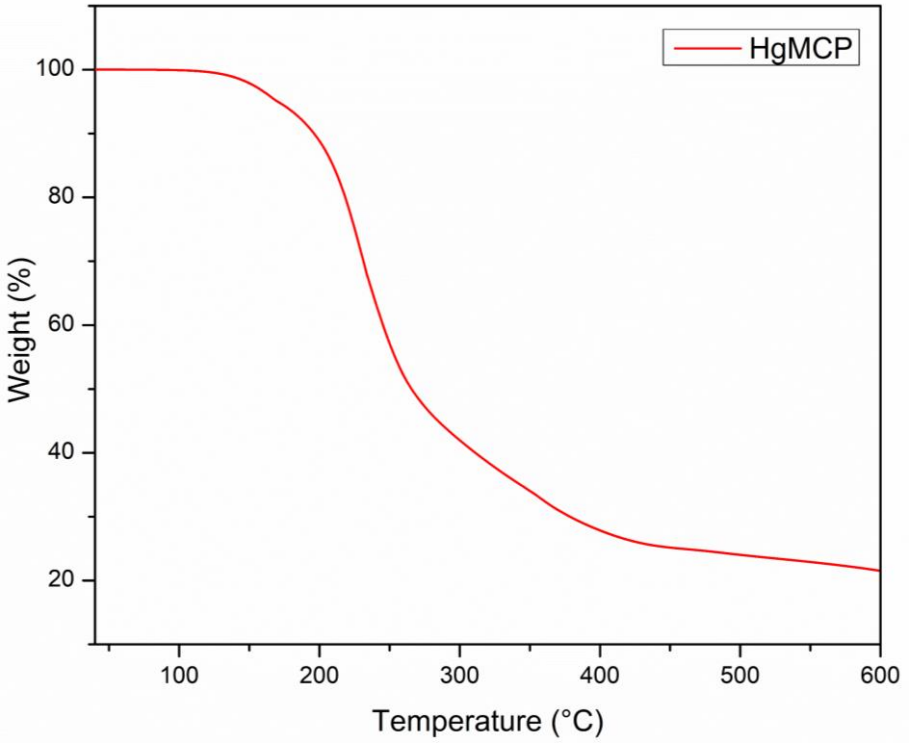


Figure S34. TGA of HgMCP.

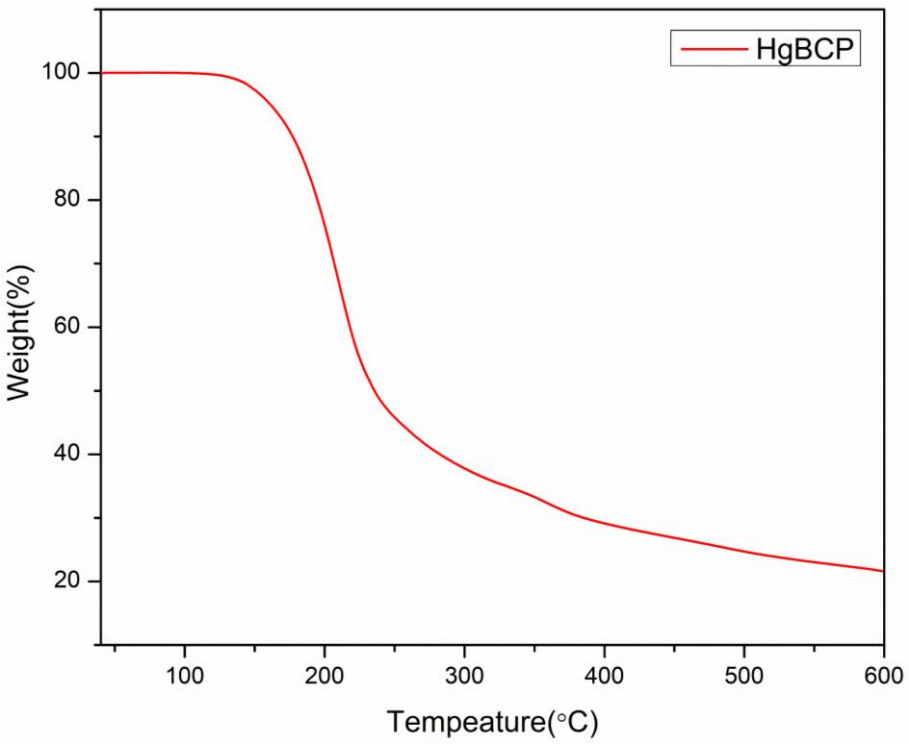


Figure S35. TGA of HgBCP.

7 IR data

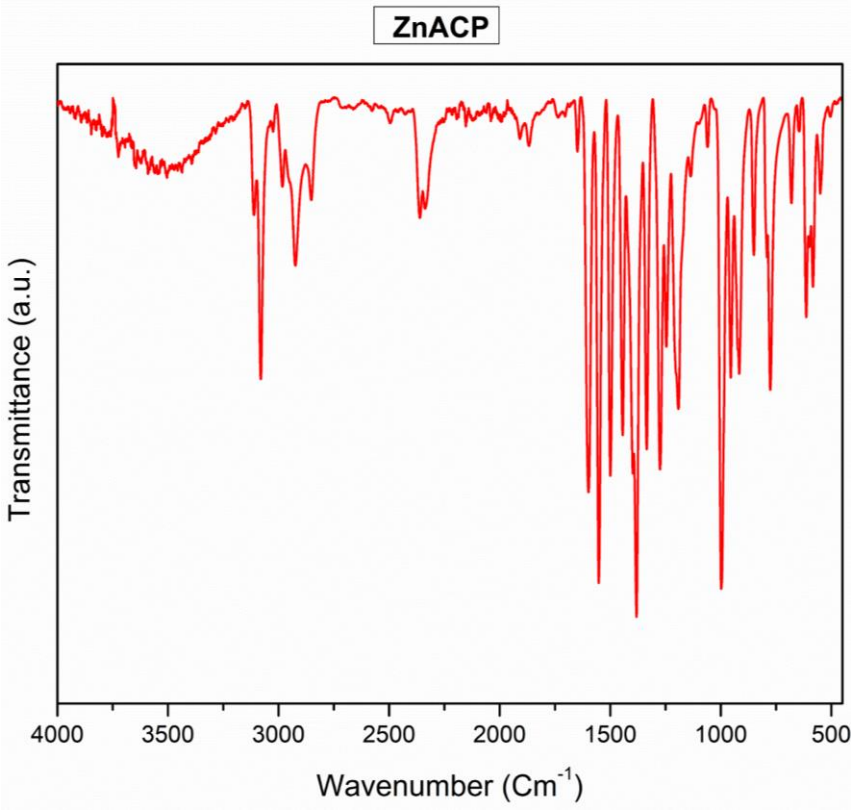


Figure S36. IR of ZnACP

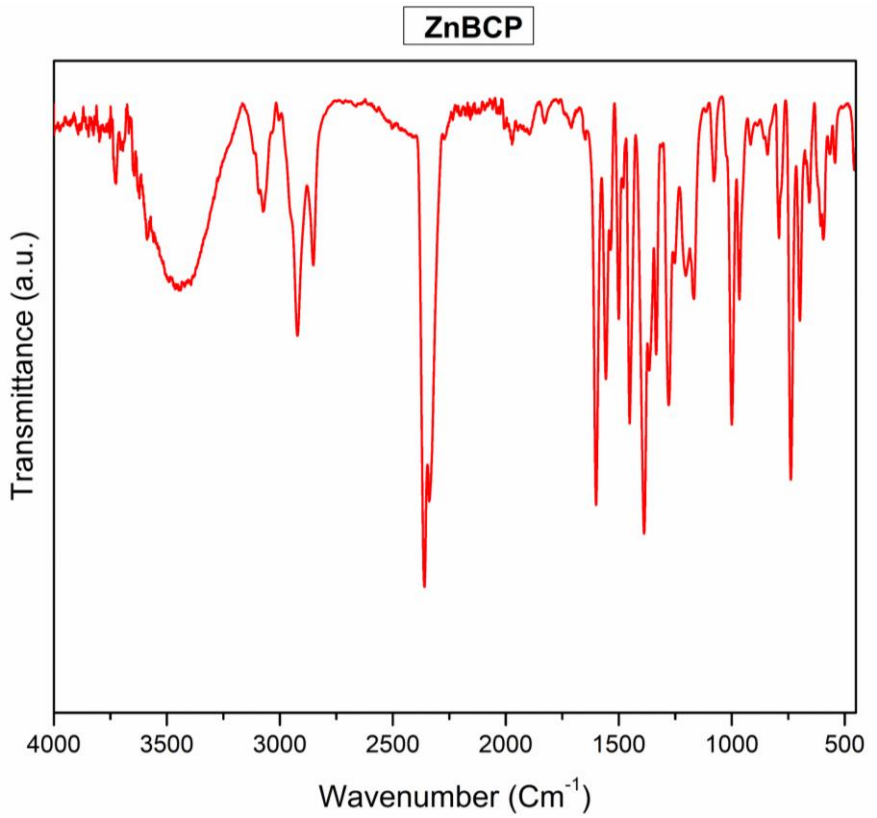


Figure S37. IR of ZnBCP.

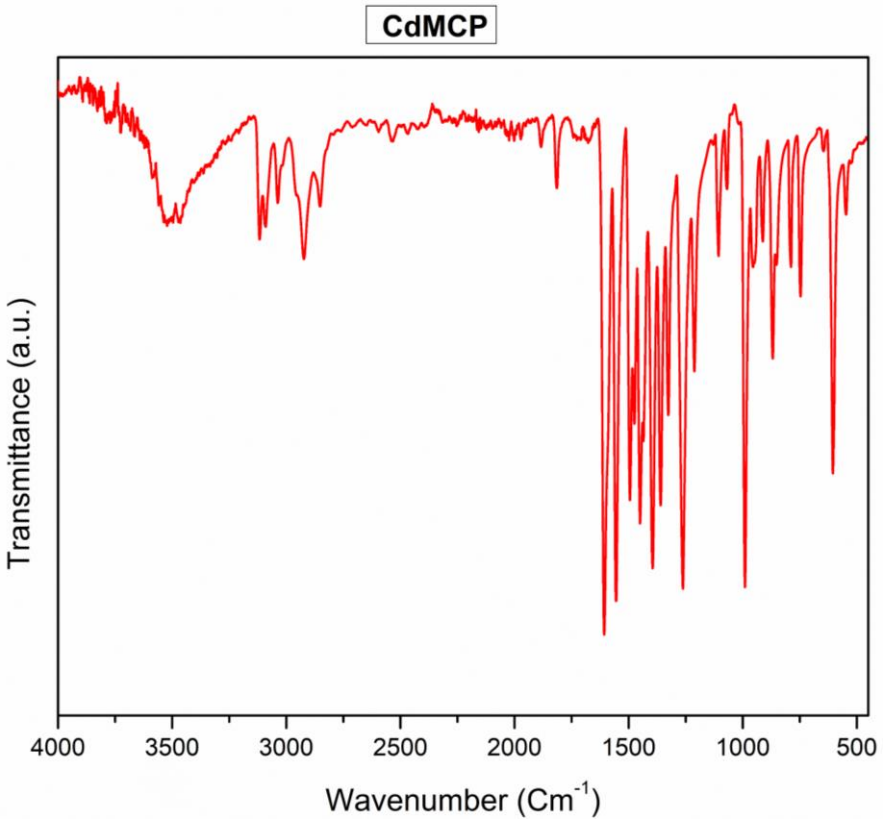


Figure S38. IR of CdMCP.

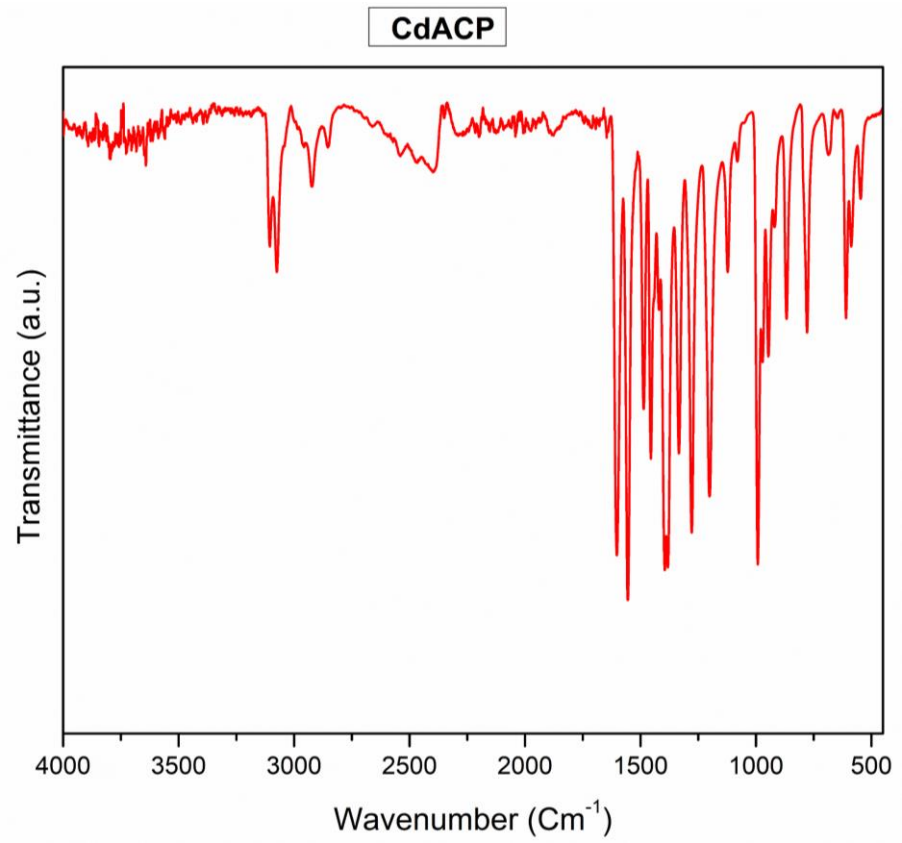


Figure S39. IR of CdACP.

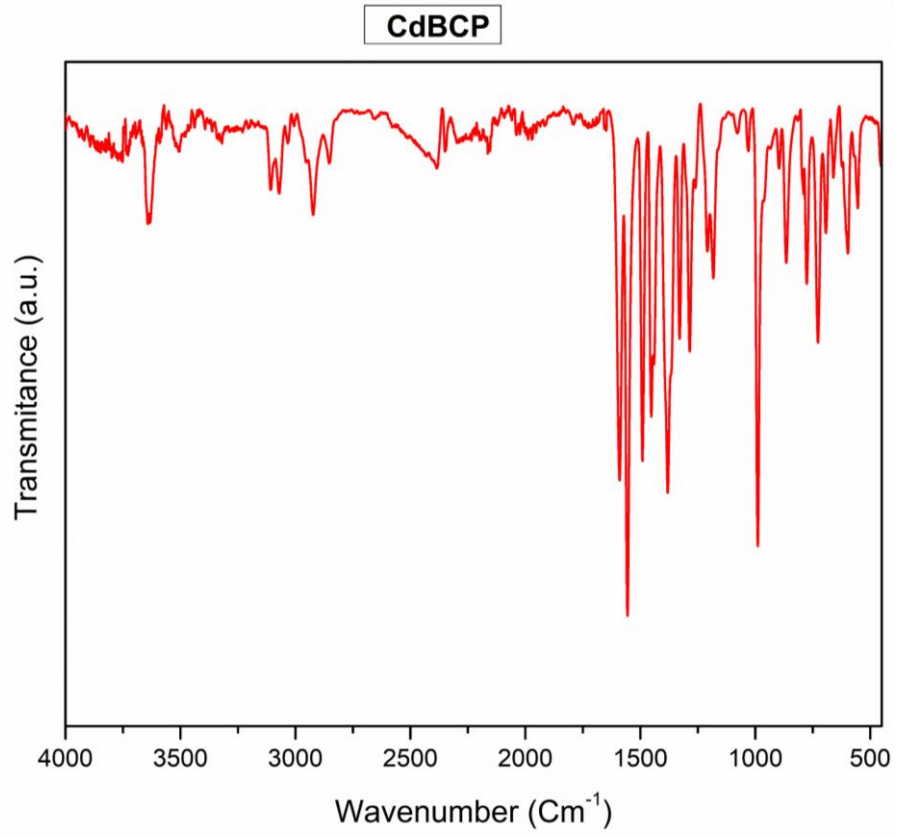


Figure S40. IR of CdBCP.

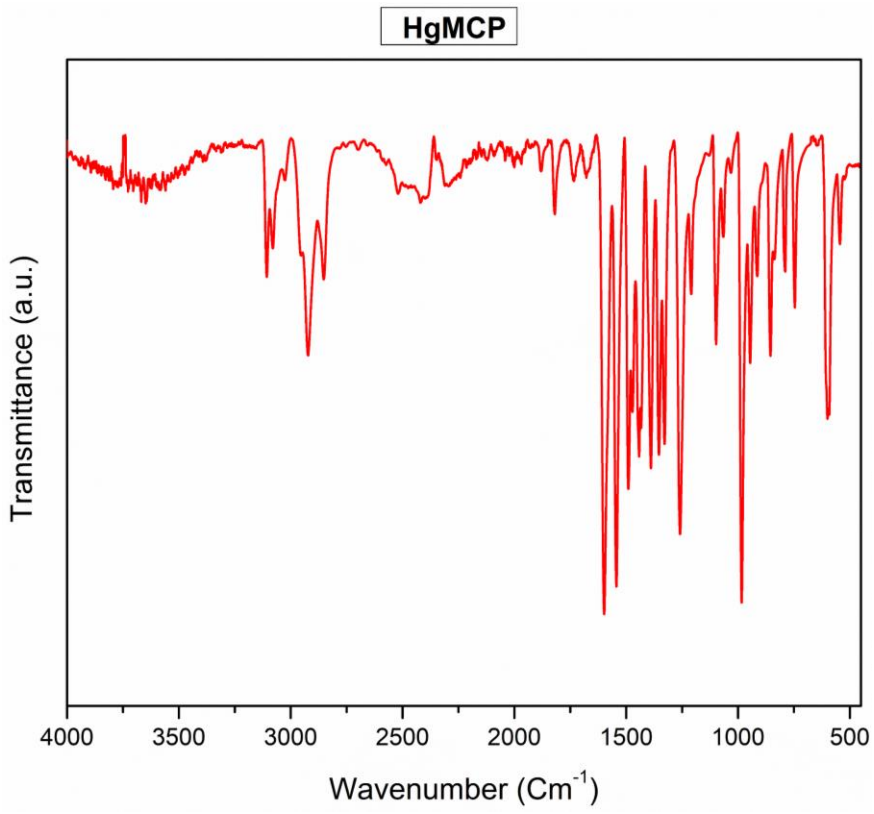


Figure S41. IR of HgMCP.

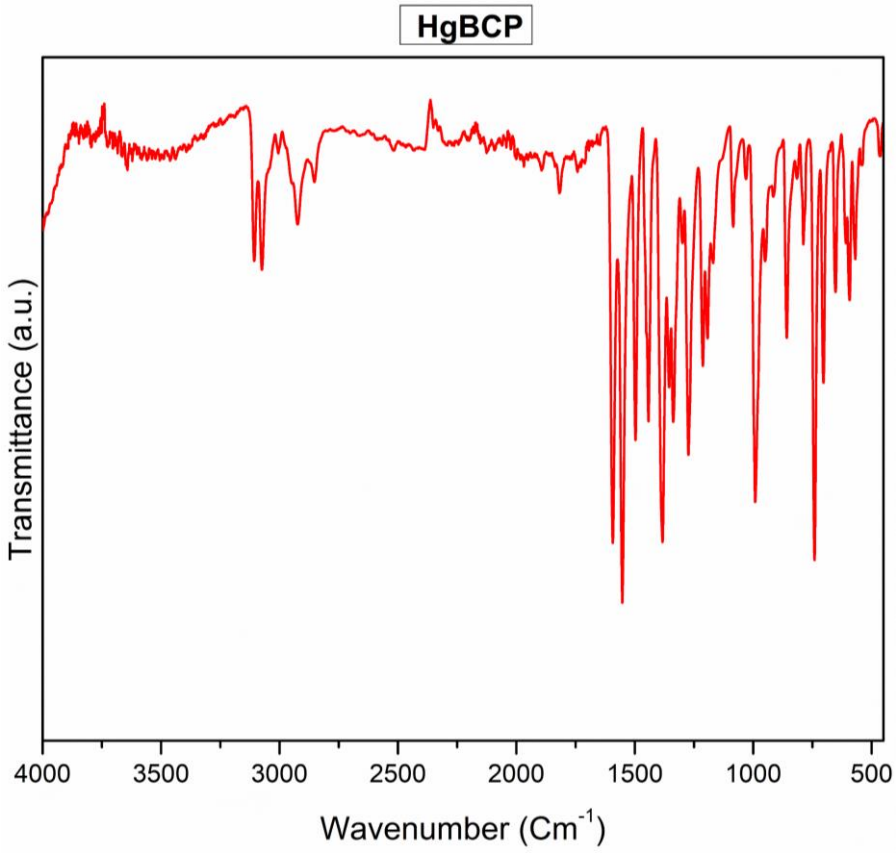


Figure S42. IR of HgBCP.

8 2-D Fingerprint region of all Compounds:

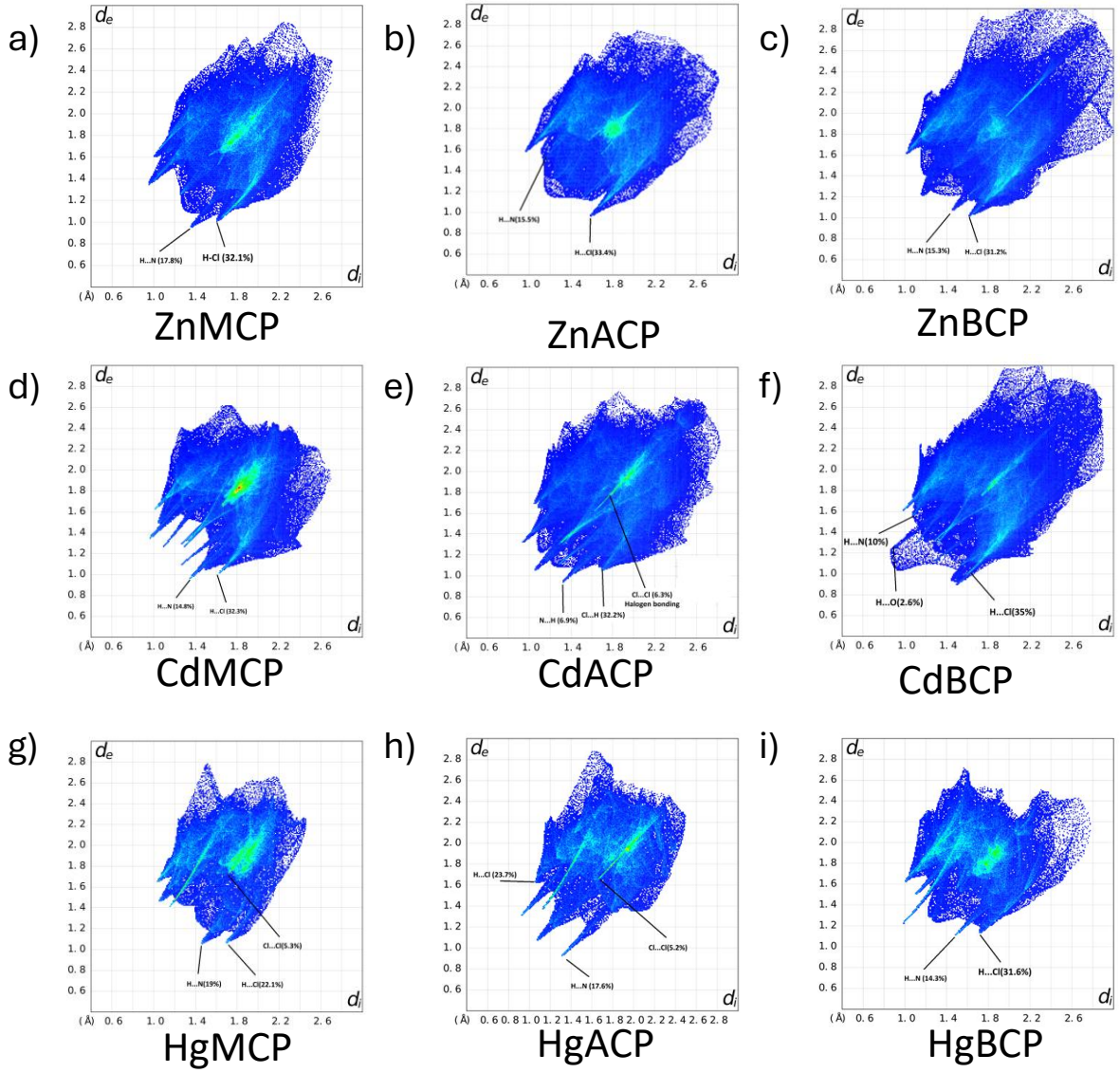


Figure S43. The 2-D Fingerprint region of (a)ZnMCP; (b)ZnACP; (c)ZnBCP; (d)CdMCP; (e)CdACP; (f)CdBCP; (g)HgMCP; (h)HgACP; (i)HgBCP.

9 BET Adsorption Studies:

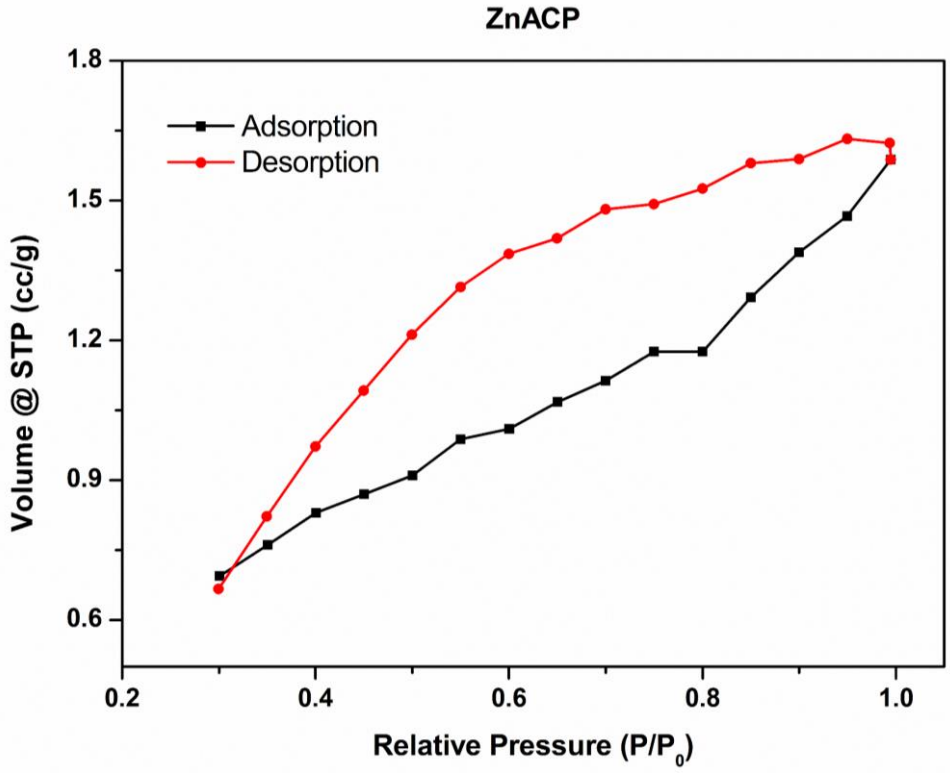


Figure S44. Adsorption and desorption studies of ZnACP at 77K.

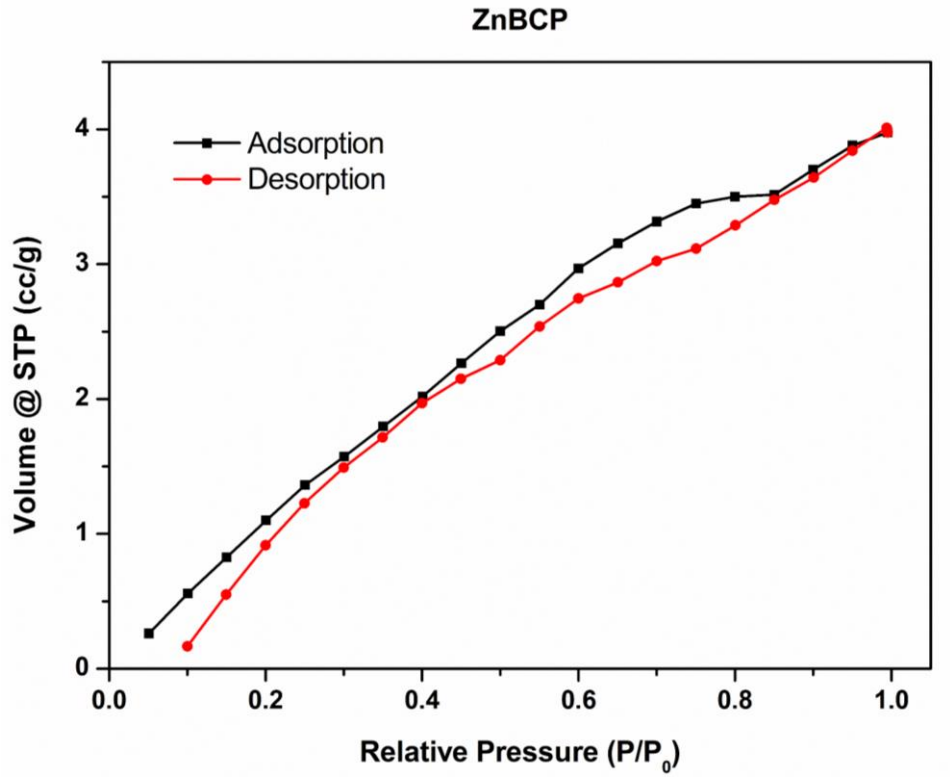


Figure S45. Adsorption and desorption studies of ZnBCP at 77K.

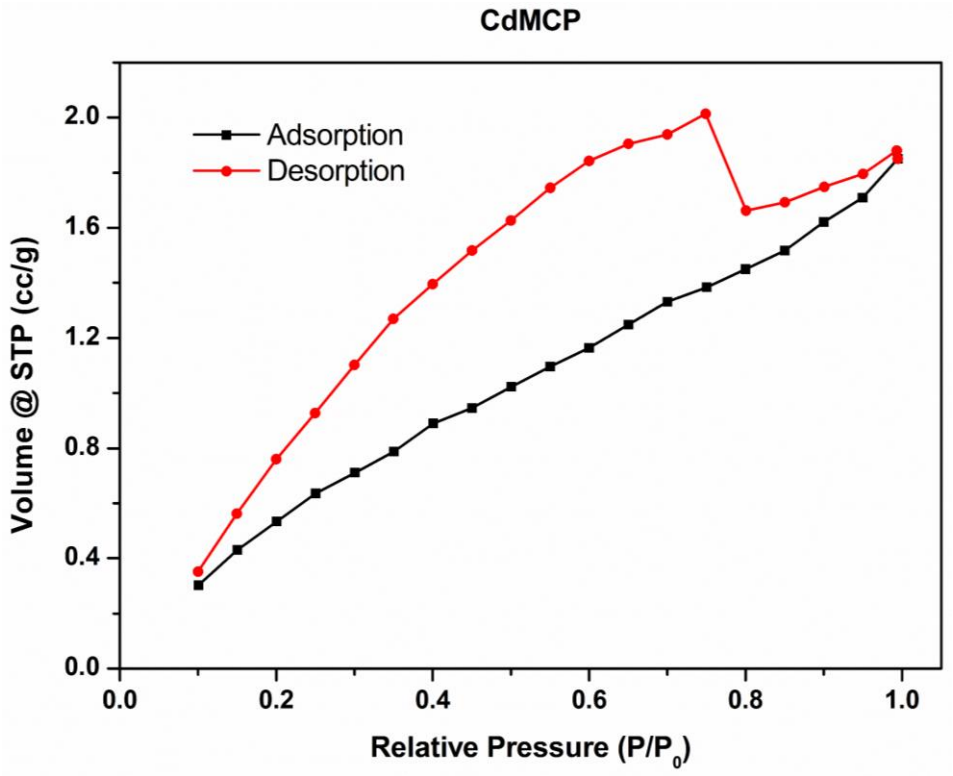


Figure S46. Adsorption and desorption studies of CdMCP at 77K.

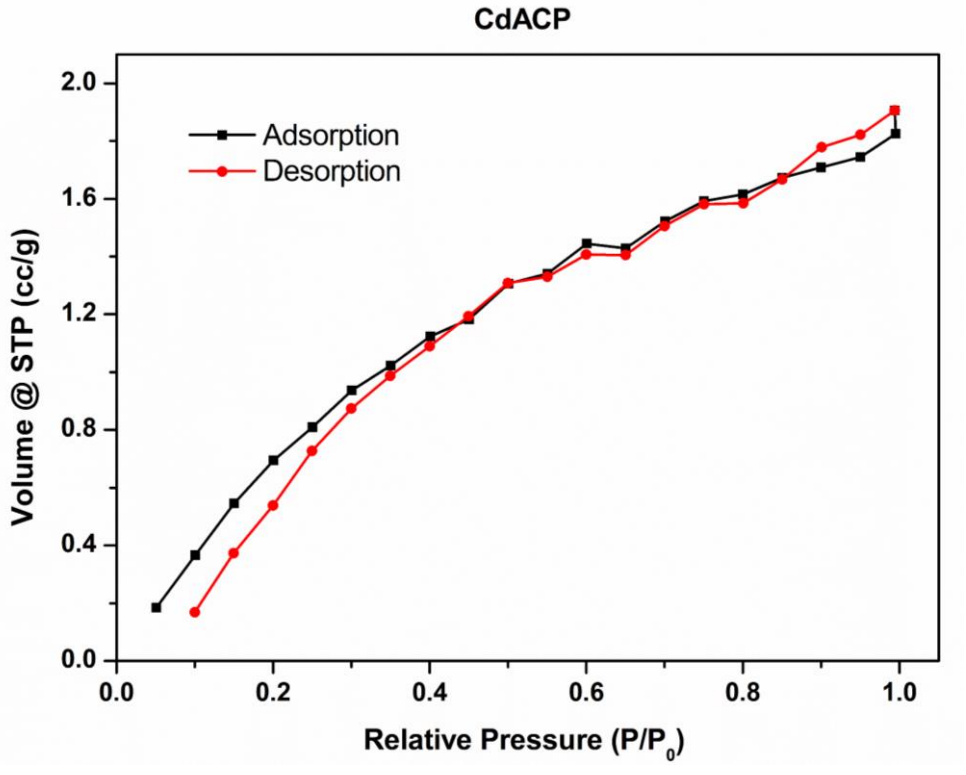


Figure S47. Adsorption and desorption studies of CdACP at 77K.

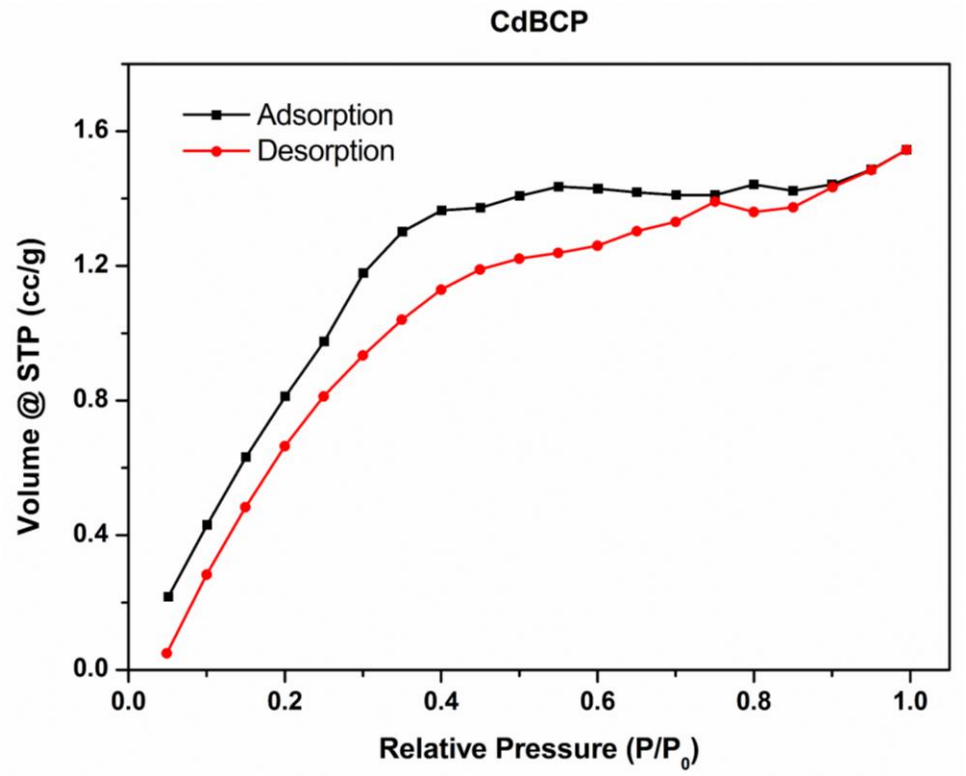


Figure S48. Adsorption and desorption studies of CdBCP at 77K.

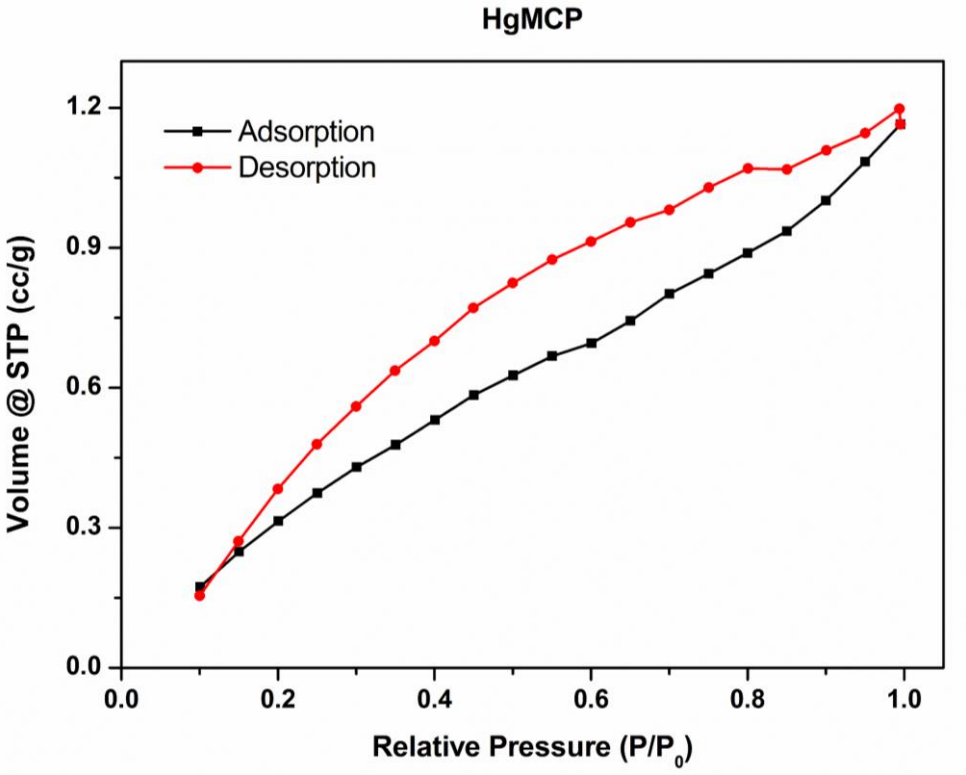


Figure S49. Adsorption and desorption studies of HgMCP at 77K.

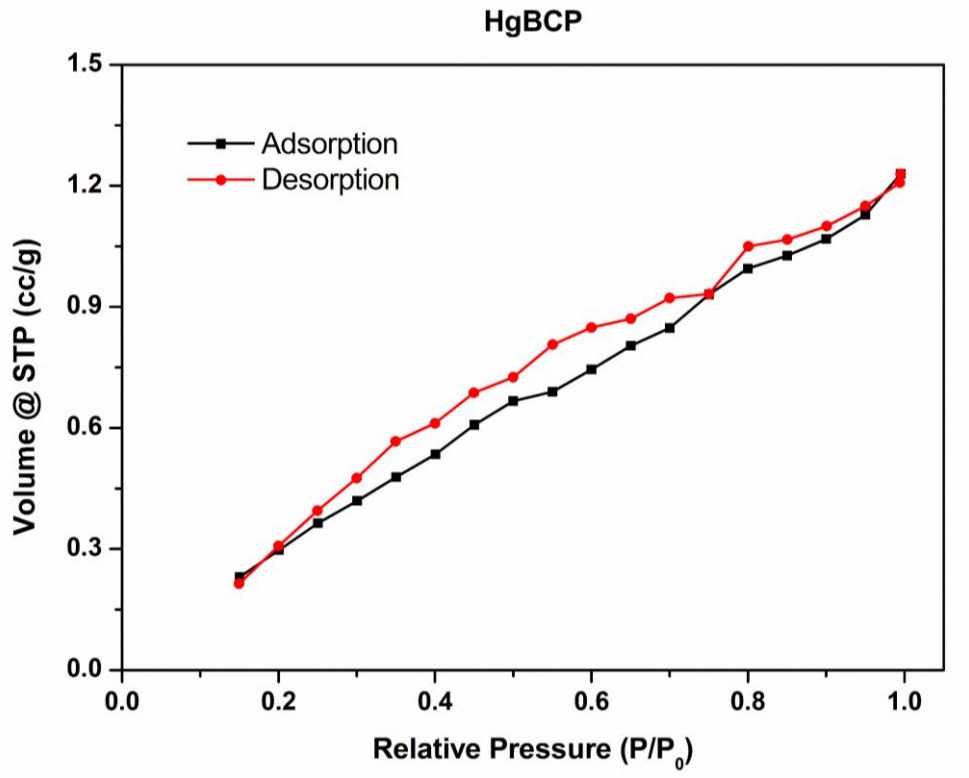


Figure S50. Adsorption and desorption studies of HgBCP at 77K.

10 Hydrogen bond, bond length, and bond angle tables.

10.1 Hydrogen bond table of ZnMCP

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(2)-H(2)...Cl(2)#1	0.95	2.70	3.427(2)	133.4
C(2")-H(2")...N(3")#2	0.95	2.65	3.510(3)	150.8
C(8)-H(8)...N(3')	0.95	2.63	3.479(3)	149.6
C(10")-H(10I)...Cl(3)	0.98	2.95	3.668(2)	130.6
C(10)-H(10B)...N(3)#3	0.98	2.39	3.306(3)	154.7
C(10')-H(10E)...N(3")#4	0.98	2.57	3.476(3)	154.3
C(10')-H(10F)...Cl(1')#5	0.98	2.82	3.803(2)	175.7
C(8")-H(8")...Cl(2)#6	0.95	2.80	3.593(2)	141.8
C(8')-H(8')...N(9")#4	0.95	2.50	3.381(3)	154.9

Symmetry transformations used to generate equivalent atoms:

#1 -x-1,-y,-z+1 #2 -x+2,-y+2,-z+2 #3 x+1,y,z

#4 x-1,y-1,z #5 -x+1,-y+1,-z+2 #6 x+1,y+1,z

10.2 Bond distance table of ZnMCP

	Bond lengths [Å]		Bond lengths [Å]		Bond lengths [Å]
Zn(1)-N(9')	2.0444(17)	N(7')-C(10')	1.470(3)	Cl(1")-C(6")	1.734(2)
Zn(1)-N(9)	2.0454(17)	N(9)-C(8)	1.331(3)	N(1")-C(6")	1.325(3)
Zn(1)-Cl(3)	2.2186(5)	N(9)-C(4)	1.379(3)	N(1")-C(2")	1.353(3)
Zn(1)-Cl(2)	2.2236(5)	N(9')-C(8')	1.332(3)	N(3")-C(2")	1.325(3)
Cl(1)-C(6)	1.731(2)	N(9')-C(4')	1.379(3)	N(3")-C(4")	1.342(3)

Cl(1')-C(6')	1.734(2)	C(2)-H(2)	0.9500	N(7")-C(8")	1.367(3)
N(1)-C(6)	1.318(3)	C(2')-H(2')	0.9500	N(7")-C(5")	1.375(3)
N(1)-C(2)	1.351(3)	C(4)-C(5)	1.403(3)	N(7")-C(10")	1.459(3)
N(1')-C(6')	1.312(3)	C(4')-C(5')	1.401(3)	N(9")-C(8")	1.309(3)
N(1')-C(2')	1.348(3)	C(5)-C(6)	1.384(3)	N(9")-C(4")	1.381(3)
N(3)-C(2)	1.331(3)	C(5')-C(6')	1.388(3)	C(2")-H(2")	0.9500
N(3)-C(4)	1.332(3)	C(8)-H(8)	0.9500	C(4")-C(5")	1.408(3)
N(3')-C(2')	1.331(3)	C(8')-H(8')	0.9500	C(5")-C(6")	1.384(3)
N(3')-C(4')	1.339(3)	C(10)-H(10A)	0.9800	C(8")-H(8")	0.9500
N(7)-C(8)	1.340(3)	C(10)-H(10B)	0.9800	C(10")-H(10G)	0.9800
N(7)-C(5)	1.384(3)	C(10)-H(10C)	0.9800	C(10")-H(10H)	0.9800
N(7)-C(10)	1.470(3)	C(10')-H(10D)	0.9800	C(10")-H(10I)	0.9800
N(7')-C(8')	1.343(3)	C(10')-H(10E)	0.9800		
N(7')-C(5')	1.381(3)	C(10')-H(10F)	0.9800		

10.3 Bond angle of ZnMCP

N(19)-Zn(1)-N(9)	97.65(7)	C(15)-N(23)-C(22)	117.44(19)	H(25B)-C(25)-H(25C)	109.5
N(19)-Zn(1)-Cl(3)	115.88(5)	N(7)-C(8)-N(9)	126.73(18)	N(30)-C(29)-N(28)	115.02(19)
N(9)-Zn(1)-Cl(3)	105.10(5)	N(7)-C(8)-C(12)	124.18(18)	N(30)-C(29)-H(29)	122.5
N(19)-Zn(1)-Cl(2)	104.81(5)	N(9)-C(8)-C(12)	109.07(17)	N(28)-C(29)-H(29)	122.5
N(9)-Zn(1)-Cl(2)	117.28(5)	N(32)-C(31)-N(30)	126.20(19)	C(29)-N(28)-C(27)	105.51(18)
Cl(3)-Zn(1)-Cl(2)	115.20(2)	N(32)-C(31)-C(27)	123.28(19)	C(29)-N(28)-C(36)	125.32(19)
C(4)-N(5)-C(6)	117.49(18)	N(30)-C(31)-C(27)	110.51(18)	C(27)-N(28)-C(36)	129.07(18)
N(21)-C(20)-N(19)	126.60(18)	C(4)-C(12)-N(11)	137.44(19)	C(22)-N(21)-C(20)	112.48(18)
N(21)-C(20)-C(16)	124.42(19)	C(4)-C(12)-C(8)	116.44(18)	C(18)-N(19)-C(20)	105.23(17)
N(19)-C(20)-C(16)	108.97(17)	N(11)-C(12)-C(8)	106.02(17)	C(18)-N(19)-Zn(1)	121.82(14)
C(18)-N(17)-C(16)	106.58(16)	N(21)-C(22)-N(23)	128.4(2)	C(20)-N(19)-Zn(1)	131.55(14)
C(18)-N(17)-C(25)	125.03(18)	N(21)-C(22)-H(22)	115.8	N(17)-C(16)-C(15)	137.25(19)
C(16)-N(17)-C(25)	128.39(17)	N(23)-C(22)-H(22)	115.8	N(17)-C(16)-C(20)	106.09(18)
N(7)-C(6)-N(5)	127.43(19)	N(28)-C(36)-H(36A)	109.5	C(15)-C(16)-C(20)	116.56(18)
N(7)-C(6)-H(6)	116.3	N(28)-C(36)-H(36B)	109.5	N(34)-C(26)-C(27)	120.78(19)
N(5)-C(6)-H(6)	116.3	H(36A)-C(36)-H(36B)	109.5	N(34)-C(26)-Cl(35)	117.59(16)
N(32)-C(33)-N(34)	128.1(2)	N(28)-C(36)-H(36C)	109.5	C(27)-C(26)-Cl(35)	121.62(16)
N(32)-C(33)-H(33)	116.0	H(36A)-C(36)-H(36C)	109.5	N(5)-C(4)-C(12)	120.90(18)
N(34)-C(33)-H(33)	116.0	H(36B)-C(36)-H(36C)	109.5	N(5)-C(4)-Cl(13)	116.74(15)
N(9)-C(10)-N(11)	113.72(18)	N(11)-C(14)-H(14A)	109.5	C(12)-C(4)-Cl(13)	122.37(16)
N(9)-C(10)-H(10)	123.1	N(11)-C(14)-H(14B)	109.5	N(19)-C(18)-N(17)	113.12(18)
N(11)-C(10)-H(10)	123.1	H(14A)-C(14)-H(14B)	109.5	N(19)-C(18)-H(18)	123.4
C(10)-N(9)-C(8)	104.89(17)	N(11)-C(14)-H(14C)	109.5	N(17)-C(18)-H(18)	123.4
C(10)-N(9)-Zn(1)	121.91(14)	H(14A)-C(14)-H(14C)	109.5	C(26)-N(34)-C(33)	117.06(18)
C(8)-N(9)-Zn(1)	131.99(14)	H(14B)-C(14)-H(14C)	109.5	C(29)-N(30)-C(31)	103.58(18)
N(23)-C(15)-C(16)	120.63(19)	C(6)-N(7)-C(8)	113.53(17)	N(28)-C(27)-C(26)	137.6(2)
N(23)-C(15)-Cl(24)	118.39(16)	N(17)-C(25)-H(25A)	109.5	N(28)-C(27)-C(31)	105.37(18)
C(16)-C(15)-Cl(24)	120.96(16)	N(17)-C(25)-H(25B)	109.5	C(26)-C(27)-C(31)	117.02(19)
C(10)-N(11)-C(12)	106.29(17)	H(25A)-C(25)-H(25B)	109.5	C(33)-N(32)-C(31)	113.75(18)
C(10)-N(11)-C(14)	125.38(18)	N(17)-C(25)-H(25C)	109.5		
C(12)-N(11)-C(14)	128.07(18)	H(25A)-C(25)-H(25C)	109.5		

10.4 Hydrogen bonds for ZnACP

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(10)-H(10A)...Cl(1)	0.97	2.89	3.3688(19)	111.3
C(2')-H(2')...Cl(3)#1	0.93	2.98	3.7196(16)	137.5
C(8')-H(8')...Cl(3)#2	0.93	2.71	3.5659(15)	153.4
C(10')-H(10C)...Cl(3)#2	0.97	3.00	3.7774(17)	138.0
C(10')-H(10D)...Cl(1')	0.97	2.90	3.3824(17)	111.7
C(10')-H(10D)...Cl(2)#3	0.97	2.93	3.7374(16)	140.9
C(11')-H(11')...Cl(2)#2	0.93	2.89	3.7315(18)	151.7

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1 #2 -x+1,-y+2,-z+1 #3 -x+2,-y+2,-z+1

10.5 Bond lengths of ZnACP

	Bond lengths [Å]		Bond lengths [Å]		Bond lengths [Å]
Zn(1)-N(9')	2.0216(13)	N(7)-C(10)	1.468(2)	C(10)-C(11)	1.501(2)
Zn(1)-N(9)	2.0300(12)	N(7')-C(8')	1.342(2)	C(10)-H(10A)	0.9700
Zn(1)-Cl(2)	2.2282(4)	N(7')-C(5')	1.387(2)	C(10)-H(10B)	0.9700
Zn(1)-Cl(3)	2.2428(4)	N(7')-C(10')	1.478(2)	C(10')-C(11')	1.500(2)
Cl(1)-C(6)	1.7297(16)	N(9)-C(8)	1.318(2)	C(10')-H(10C)	0.9700
Cl(1')-C(6')	1.7308(17)	N(9)-C(4)	1.3802(19)	C(10')-H(10D)	0.9700
N(1)-C(6)	1.316(2)	N(9')-C(8')	1.329(2)	C(11)-C(12)	1.317(3)
N(1)-C(2)	1.354(2)	N(9')-C(4')	1.3793(19)	C(11)-H(11)	0.9300
N(1')-C(6')	1.320(2)	C(2)-H(2)	0.9300	C(11')-C(12')	1.319(3)
N(1')-C(2')	1.353(2)	C(2')-H(2')	0.9300	C(11')-H(11')	0.9300
N(3)-C(2)	1.328(2)	C(4)-C(5)	1.401(2)	C(12)-H(12A)	0.9300
N(3)-C(4)	1.335(2)	C(4')-C(5')	1.400(2)	C(12)-H(12B)	0.9300
N(3')-C(2')	1.332(2)	C(5)-C(6)	1.393(2)	C(12')-H(12C)	0.9300
N(3')-C(4')	1.340(2)	C(5')-C(6')	1.382(2)	C(12')-H(12D)	0.9300
N(7)-C(8)	1.3537(19)	C(8)-H(8)	0.9300		
N(7)-C(5)	1.384(2)	C(8')-H(8')	0.9300		

10.6 Bond angles of ZnACP

	angles [°]		angles [°]		angles [°]
N(9')-Zn(1)-N(9)	101.21(5)	N(3)-C(4)-N(9)	126.18(14)	N(1')-C(2')-H(2')	116.1
N(9')-Zn(1)-Cl(2)	104.69(4)	N(3)-C(4)-C(5)	125.00(14)	N(3)-C(4)-N(9)	126.18(14)
N(9)-Zn(1)-Cl(2)	116.99(4)	N(9)-C(4)-C(5)	108.81(14)	N(3)-C(4)-C(5)	125.00(14)
N(9')-Zn(1)-Cl(3)	114.21(4)	N(3')-C(4')-N(9')	126.26(14)	N(9)-C(4)-C(5)	108.81(14)
N(9)-Zn(1)-Cl(3)	102.30(4)	N(3')-C(4')-C(5')	124.68(14)	N(3')-C(4')-N(9')	126.26(14)
Cl(2)-Zn(1)-Cl(3)	116.732(15)	N(9')-C(4')-C(5')	109.04(13)	N(3')-C(4')-C(5')	124.68(14)
C(6)-N(1)-C(2)	117.72(14)	N(7)-C(5)-C(6)	137.70(15)	N(9')-C(4')-C(5')	109.04(13)
C(6')-N(1')-C(2')	117.48(14)	N(7)-C(5)-C(4)	106.20(13)	N(7)-C(5)-C(6)	137.70(15)
C(2)-N(3)-C(4)	112.80(14)	C(6)-C(5)-C(4)	116.10(15)	N(7)-C(5)-C(4)	106.20(13)
C(2')-N(3')-C(4')	112.80(14)	C(6')-C(5')-N(7')	137.44(15)	C(6)-C(5)-C(4)	116.10(15)
C(8)-N(7)-C(5)	106.05(13)	C(6')-C(5')-C(4')	116.36(14)	C(6')-C(5')-N(7')	137.44(15)
C(8)-N(7)-C(10)	125.29(14)	N(7')-C(5')-C(4')	106.13(13)	C(6')-C(5')-C(4')	116.36(14)
C(5)-N(7)-C(10)	128.32(13)	N(1)-C(6)-C(5)	120.53(14)	N(7')-C(5')-C(4')	106.13(13)
C(8')-N(7')-C(5')	106.13(12)	N(1)-C(6)-Cl(1)	117.44(12)	N(1)-C(6)-C(5)	120.53(14)
C(8')-N(7')-C(10')	124.09(13)	C(5)-C(6)-Cl(1)	122.01(13)	N(1)-C(6)-Cl(1)	117.44(12)
C(5')-N(7')-C(10')	129.76(13)	N(1')-C(6')-C(5')	120.91(15)	C(5)-C(6)-Cl(1)	122.01(13)
C(8)-N(9)-C(4)	105.58(12)	N(1')-C(6')-Cl(1')	117.14(12)	N(1')-C(6')-C(5')	120.91(15)
C(8)-N(9)-Zn(1)	127.59(11)	C(5')-C(6')-Cl(1')	121.93(13)	N(1')-C(6')-Cl(1')	117.14(12)
C(4)-N(9)-Zn(1)	125.56(10)	N(9)-C(8)-N(7)	113.32(14)	C(5')-C(6')-Cl(1')	121.93(13)
C(8')-N(9')-C(4')	105.04(13)	N(9)-C(8)-H(8)	123.3	N(9)-C(8)-N(7)	113.32(14)
C(8')-N(9')-Zn(1)	124.29(10)	N(9')-C(8')-N(7')	113.65(13)	N(9)-C(8)-H(8)	123.3

C(4')-N(9')-Zn(1)	130.49(11)	N(9')-C(8')-H(8')	123.2	N(9')-C(8')-N(7')	113.65(13)
N(3)-C(2)-N(1)	127.84(16)	N(7)-C(10)-C(11)	111.95(14)	N(9')-C(8')-H(8')	123.2
N(3)-C(2)-H(2)	116.1	N(7)-C(10)-H(10A)	109.2	N(7)-C(10)-C(11)	111.95(14)
N(1)-C(2)-H(2)	116.1	C(11)-C(10)-H(10B)	109.2	N(7)-C(10)-H(10A)	109.2
N(3')-C(2')-N(1')	127.74(15)	H(10A)-C(10)-H(10B)	107	N(7)-C(10)-H(10B)	109.2

10.7 Hydrogen bonds for ZnBCP

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(8A)-H(8A)...N(3B)	0.93	2.64	3.383(6)	137.4
C(10)-H(10B)...Cl(1)	0.97	2.84	3.399(8)	117.2
C(10A)-H(10C)...Cl(1A)	0.97	2.80	3.372(5)	118.7
C(2B)-H(2B)...Cl(08)	0.93	2.86	3.653(5)	143.7
C(8B)-H(8B)...Cl(04)#1	0.93	2.75	3.523(4)	141.3
C(8C)-H(8C)...Cl(03)#2	0.93	2.82	3.627(5)	145.2
C(10B)-H(10E)...Cl(1B)	0.97	2.88	3.385(5)	113.3
C(10B)-H(10F)...Cl(04)#1	0.97	2.78	3.682(5)	155.3

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1 #2 -x,-y+1,-z+1

10.8 Bond length of ZnBCP

	Bond lengths [Å]		Bond lengths [Å]		Bond lengths [Å]
Zn(1)-N(9A)	2.017(4)	N(9)-C(8)	1.331(7)	C(11A)-C(16A)	1.360(6)
Zn(1)-N(9)	2.033(4)	N(9)-C(4)	1.366(7)	C(11A)-C(12A)	1.396(6)
Zn(1)-Cl(06)	2.1946(15)	N(9A)-C(8A)	1.320(6)	C(12)-C(13)	1.401(10)
Zn(1)-Cl(08)	2.2169(17)	N(9A)-C(4A)	1.377(6)	C(12)-H(12)	0.9300
Cl(1)-C(6)	1.717(7)	C(2)-H(2)	0.9300	C(12A)-C(13A)	1.396(7)
Cl(1A)-C(6A)	1.736(6)	C(2A)-H(2A)	0.9300	C(12A)-H(12A)	0.9300
N(1)-C(6)	1.321(9)	C(4)-C(5)	1.416(7)	C(13)-C(14)	1.376(11)
N(1)-C(2)	1.372(10)	C(4A)-C(5A)	1.386(7)	C(13)-H(13)	0.9300
N(1A)-C(6A)	1.318(7)	C(5)-C(6)	1.365(8)	C(13A)-C(14A)	1.351(8)
N(1A)-C(2A)	1.332(8)	C(5A)-C(6A)	1.370(7)	C(13A)-H(13A)	0.9300
N(3)-C(2)	1.308(8)	C(8)-H(8)	0.9300	C(14)-C(15)	1.328(11)
N(3)-C(4)	1.334(7)	C(8A)-H(8A)	0.9300	C(14)-H(14)	0.9300
N(3A)-C(2A)	1.312(7)	C(10)-C(11)	1.485(10)	C(14A)-C(15A)	1.381(8)
N(3A)-C(4A)	1.345(6)	C(10)-H(10A)	0.9700	C(14A)-H(14A)	0.9300
N(7)-C(8)	1.340(7)	C(10)-H(10B)	0.9700	C(15)-C(16)	1.373(11)
N(7)-C(5)	1.351(8)	C(10A)-C(11A)	1.511(6)	C(15)-H(15)	0.9300
N(7)-C(10)	1.504(8)	C(10A)-H(10C)	0.9700	C(15A)-C(16A)	1.414(7)
N(7A)-C(8A)	1.326(6)	C(10A)-H(10D)	0.9700	C(15A)-H(15A)	0.9300
N(7A)-C(5A)	1.384(5)	C(11)-C(12)	1.380(9)	C(16)-H(16)	0.9300
N(7A)-C(10A)	1.472(6)	C(11)-C(16)	1.396(10)	C(16A)-H(16A)	0.9300

10.9 Bond angles of ZnBCP

	angles [°]		angles [°]		angles [°]
N(9A)-Zn(1)-N(9)	102.96(17)	N(7)-C(5)-C(6)	137.3(6)	C(16A)-C(11A)-C(10A)	123.9(4)
N(9A)-Zn(1)-Cl(06)	117.01(12)	N(7)-C(5)-C(4)	105.9(5)	C(12A)-C(11A)-C(10A)	116.8(4)
N(9)-Zn(1)-Cl(06)	106.89(14)	C(6)-C(5)-C(4)	116.7(6)	C(11)-C(12)-C(13)	119.9(7)
N(9A)-Zn(1)-Cl(08)	104.89(12)	C(6A)-C(5A)-N(7A)	138.2(5)	C(11)-C(12)-H(12)	120.0
N(9)-Zn(1)-Cl(08)	109.52(16)	C(6A)-C(5A)-C(4A)	116.7(4)	C(13)-C(12)-H(12)	120.0
Cl(06)-Zn(1)-Cl(08)	114.84(8)	N(7A)-C(5A)-C(4A)	105.1(4)	C(13A)-C(12A)-C(11A)	120.2(5)
C(6)-N(1)-C(2)	118.0(6)	N(1)-C(6)-C(5)	119.8(6)	C(13A)-C(12A)-H(12A)	119.9
C(6A)-N(1A)-C(2A)	118.0(5)	N(1)-C(6)-Cl(1)	115.9(5)	C(11A)-C(12A)-H(12A)	119.9
C(2)-N(3)-C(4)	112.3(6)	C(5)-C(6)-Cl(1)	124.2(5)	C(14)-C(13)-C(12)	120.4(7)
C(2A)-N(3A)-C(4A)	112.7(5)	N(1A)-C(6A)-C(5A)	120.3(5)	C(14)-C(13)-H(13)	119.8
C(8)-N(7)-C(5)	107.1(5)	N(1A)-C(6A)-Cl(1A)	117.8(4)	C(12)-C(13)-H(13)	119.8
C(8)-N(7)-C(10)	123.3(6)	C(5A)-C(6A)-Cl(1A)	121.9(4)	C(14A)-C(13A)-C(12A)	120.3(5)
C(5)-N(7)-C(10)	129.5(5)	N(9)-C(8)-N(7)	113.3(5)	C(14A)-C(13A)-H(13A)	119.9

C(8A)-N(7A)-C(5A)	107.0(4)	N(9)-C(8)-H(8)	123.3	C(12A)-C(13A)-H(13A)	119.9
C(8A)-N(7A)-C(10A)	124.2(4)	N(7)-C(8)-H(8)	123.3	C(15)-C(14)-C(13)	119.8(8)
C(5A)-N(7A)-C(10A)	128.8(4)	N(9A)-C(8A)-N(7A)	113.6(4)	C(15)-C(14)-H(14)	120.1
C(8)-N(9)-C(4)	104.6(5)	N(9A)-C(8A)-H(8A)	123.2	C(13)-C(14)-H(14)	120.1
C(8)-N(9)-Zn(1)	126.3(4)	N(7A)-C(8A)-H(8A)	123.2	C(13A)-C(14A)-C(15A)	120.5(5)
C(4)-N(9)-Zn(1)	128.8(4)	C(11)-C(10)-N(7)	111.8(5)	C(13A)-C(14A)-H(14A)	119.7
C(8A)-N(9A)-C(4A)	104.5(4)	C(11)-C(10)-H(10A)	109.3	C(15A)-C(14A)-H(14A)	119.7
C(8A)-N(9A)-Zn(1)	127.1(3)	N(7)-C(10)-H(10A)	109.3	C(14)-C(15)-C(16)	121.0(8)
C(4A)-N(9A)-Zn(1)	127.3(3)	C(11)-C(10)-H(10B)	109.3	C(14)-C(15)-H(15)	119.5
N(3)-C(2)-N(1)	127.9(7)	N(7)-C(10)-H(10B)	109.3	C(16)-C(15)-H(15)	119.5
N(3)-C(2)-H(2)	116.0	H(10A)-C(10)-H(10B)	107.9	C(14A)-C(15A)-C(16A)	119.4(5)
N(1)-C(2)-H(2)	116.0	N(7A)-C(10A)-C(11A)	113.6(4)	C(14A)-C(15A)-H(15A)	120.3
N(3A)-C(2A)-N(1A)	128.0(5)	N(7A)-C(10A)-H(10C)	108.8	C(16A)-C(15A)-H(15A)	120.3
N(3A)-C(2A)-H(2A)	116.0	C(11A)-C(10A)-H(10C)	108.8	C(15)-C(16)-C(11)	121.5(7)
N(1A)-C(2A)-H(2A)	116.0	N(7A)-C(10A)-H(10D)	108.8	C(15)-C(16)-H(16)	119.2
N(3)-C(4)-N(9)	125.8(5)	C(11A)-C(10A)-H(10D)	108.8	C(11)-C(16)-H(16)	119.2
N(3)-C(4)-C(5)	125.1(5)	H(10C)-C(10A)-H(10D)	107.7	C(11A)-C(16A)-C(15A)	120.3(5)
N(9)-C(4)-C(5)	109.0(5)	C(12)-C(11)-C(16)	117.2(7)	C(11A)-C(16A)-H(16A)	119.9
N(3A)-C(4A)-N(9A)	125.8(5)	C(12)-C(11)-C(10)	120.8(7)	C(15A)-C(16A)-H(16A)	119.9
N(3A)-C(4A)-C(5A)	124.3(4)	C(16)-C(11)-C(10)	121.9(6)		
N(9A)-C(4A)-C(5A)	109.9(4)	C(16A)-C(11A)-C(12A)	119.3(4)		

10.10 Hydrogen bonds for CdMCP

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(2)-H(2)...Cl(3)#3	0.93	2.87	3.398(6)	117.3
C(8)-H(8)...Cl(1)#5	0.93	2.81	3.741(6)	175.1
C(10)-H(10A)...Cl(3)#6	0.96	2.97	3.738(6)	138.3
C(10)-H(10B)...N(1)#5	0.96	2.44	3.347(8)	156.8
C(10)-H(10C)...N(3)#7	0.96	2.67	3.520(8)	147.7

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+2,-z+1 #2 -x+3/2,y,-z+1 #3 x-1/2,-y+2,z

#4 x+1/2,-y+2,z #5 x+1/2,-y+1,z #6 -x+3/2,y-1,-z+1

#7 -x+1,y-1/2,-z+1/2

10.11 Bond lengths of CdMCP:

	Bond lengths [Å]		Bond lengths [Å]
Cd(1)-N(3)	2.380(5)	N(3)-C(2)	1.340(8)
Cd(1)-N(3)#1	2.380(5)	N(3)-C(4)	1.352(7)
Cd(1)-Cl(2)	2.5860(12)	N(7)-C(8)	1.351(8)
Cd(1)-Cl(2)#1	2.5861(12)	N(7)-C(5)	1.369(7)
Cd(1)-Cl(3)#2	2.6492(13)	N(7)-C(10)	1.479(7)
Cd(1)-Cl(3)#3	2.6492(13)	N(9)-C(8)	1.336(8)
Cd(2)-N(9)	2.416(5)	N(9)-C(4)	1.375(7)
Cd(2)-N(9)#2	2.416(5)	C(2)-H(2)	0.9300
Cd(2)-Cl(3)	2.6068(13)	C(4)-C(5)	1.408(8)
Cd(2)-Cl(3)#2	2.6068(13)	C(5)-C(6)	1.382(8)
Cd(2)-Cl(2)#1	2.6086(12)	C(8)-H(8)	0.9300
Cd(2)-Cl(2)#4	2.6086(12)	C(10)-H(10A)	0.9600
Cl(1)-C(6)	1.788(6)	C(10)-H(10B)	0.9600
N(1)-C(6)	1.313(8)	C(10)-H(10C)	0.9600

N(1)-C(2)	1.355(8)		

10.12 Angles for CdMCP:

	angles [°]		angles [°]		Angles[°]
N(3)-Cd(1)-N(3)#1	180.0	N(9)-Cd(2)-Cl(2)#1	87.45(11)	N(3)-C(2)-N(1)	127.8(5)
N(3)-Cd(1)-Cl(2)	92.67(11)	N(9)#2-Cd(2)-Cl(2)#1	90.61(11)	N(3)-C(2)-H(2)	116.1
N(3)#1-Cd(1)-Cl(2)	87.33(11)	Cl(3)-Cd(2)-Cl(2)#1	95.61(4)	N(1)-C(2)-H(2)	116.1
N(3)-Cd(1)-Cl(2)#1	87.33(11)	Cl(3)#2-Cd(2)-Cl(2)#1	85.97(4)	N(3)-C(4)-N(9)	127.7(5)
N(3)#1-Cd(1)-Cl(2)#1	92.67(11)	N(9)-Cd(2)-Cl(2)#4	90.61(11)	N(3)-C(4)-C(5)	122.7(5)
Cl(2)-Cd(1)-Cl(2)#1	180.00(5)	N(9)#2-Cd(2)-Cl(2)#4	87.46(11)	N(9)-C(4)-C(5)	109.6(5)
N(3)-Cd(1)-Cl(3)#2	91.38(12)	Cl(3)-Cd(2)-Cl(2)#4	85.97(4)	N(7)-C(5)-C(6)	135.9(5)
N(3)#1-Cd(1)-Cl(3)#2	88.62(12)	Cl(3)#2-Cd(2)-Cl(2)#4	95.61(4)	N(7)-C(5)-C(4)	106.2(5)
Cl(2)-Cd(1)-Cl(3)#2	94.45(4)	Cl(2)#1-Cd(2)-Cl(2)#4	177.42(6)	C(6)-C(5)-C(4)	117.8(5)
Cl(2)#1-Cd(1)-Cl(3)#2	85.55(4)	Cd(1)-Cl(2)-Cd(2)#1	91.83(4)	N(1)-C(6)-C(5)	120.6(5)
N(3)-Cd(1)-Cl(3)#3	88.62(12)	Cd(2)-Cl(3)-Cd(1)#2	90.46(4)	N(1)-C(6)-Cl(1)	117.4(4)
N(3)#1-Cd(1)-Cl(3)#3	91.38(12)	C(6)-N(1)-C(2)	117.6(5)	C(5)-C(6)-Cl(1)	122.0(4)
Cl(2)-Cd(1)-Cl(3)#3	85.55(4)	C(2)-N(3)-C(4)	113.3(5)	N(9)-C(8)-N(7)	113.7(5)
Cl(2)#1-Cd(1)-Cl(3)#3	94.45(4)	C(2)-N(3)-Cd(1)	116.5(4)	N(9)-C(8)-H(8)	123.1
Cl(3)#2-Cd(1)-Cl(3)#3	180.0	C(4)-N(3)-Cd(1)	129.3(4)	N(7)-C(8)-H(8)	123.1
N(9)-Cd(2)-N(9)#2	83.1(2)	C(8)-N(7)-C(5)	106.3(5)	N(7)-C(10)-H(10A)	109.5
N(9)-Cd(2)-Cl(3)	168.70(12)	C(8)-N(7)-C(10)	126.4(5)	N(7)-C(10)-H(10B)	109.5
N(9)#2-Cd(2)-Cl(3)	86.03(11)	C(5)-N(7)-C(10)	127.3(5)	H(10A)-C(10)-H(10B)	109.5
N(9)-Cd(2)-Cl(3)#2	86.03(11)	C(8)-N(9)-C(4)	104.3(5)	N(7)-C(10)-H(10C)	109.5
N(9)#2-Cd(2)-Cl(3)#2	168.70(12)	C(8)-N(9)-Cd(2)	121.0(4)	H(10A)-C(10)-H(10C)	109.5
Cl(3)-Cd(2)-Cl(3)#2	105.01(6)	C(4)-N(9)-Cd(2)	131.9(4)	H(10B)-C(10)-H(10C)	109.5

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+2,-z+1 #2 -x+3/2,y,-z+1 #3 x-1/2,-y+2,z

#4 x+1/2,-y+2,z

10.13 Hydrogen bond table for CdACP

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(2)-H(2)...Cl(3)#1	0.93	2.86	3.546(9)	131.3
C(2')-H(2')...Cl(4)#2	0.93	2.85	3.463(9)	124.8
C(8)-H(8)...Cl(5)	0.93	2.78	3.377(8)	122.6
C(8)-H(8)...N(1')#3	0.93	2.58	3.375(10)	144.3
C(8')-H(8')...N(1)#4	0.93	2.40	3.263(11)	154.7
C(10)-H(10A)...Cl(1)	0.97	2.83	3.322(8)	112.5
C(10)-H(10A)...Cl(3)#5	0.97	2.81	3.450(9)	124.4
C(10)-H(10B)...N(1')#3	0.97	2.54	3.430(11)	152.9
C(11)-H(11)...Cl(1)	0.93	2.97	3.506(9)	117.8
C(11')-H(11')...Cl(1')	0.93	2.93	3.451(10)	116.5

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z+1 #2 -x,-y+1,-z+2 #3 -x+1,-y+1,-z+2

#4 -x+1,-y+1,-z+1 #5 x+1,y,z

10.14 Bond lengths of CdACP:

Cd(1)-N(3)#1	2.397(7)	N(1)-C(6)	1.327(11)	C(4)-C(5)	1.404(12)
Cd(1)-N(3)	2.397(7)	N(1)-C(2)	1.343(11)	C(4')-C(5')	1.400(11)
Cd(1)-Cl(2)	2.5852(19)	N(1')-C(2')	1.328(12)	C(5)-C(6)	1.386(12)
Cd(1)-Cl(2)#1	2.5852(19)	N(1')-C(6')	1.336(12)	C(5')-C(6')	1.382(11)
Cd(1)-Cl(3)	2.6436(19)	N(3)-C(2)	1.315(11)	C(8)-H(8)	0.9300
Cd(1)-Cl(3)#1	2.6436(19)	N(3)-C(4)	1.342(10)	C(8')-H(8')	0.9300
Cd(2)-N(9')	2.366(7)	N(3')-C(2')	1.330(10)	C(10)-C(11)	1.491(12)
Cd(2)-N(9)	2.398(7)	N(3')-C(4')	1.340(11)	C(10)-H(10A)	0.9700
Cd(2)-Cl(4)	2.612(2)	N(7)-C(8)	1.331(11)	C(10)-H(10B)	0.9700
Cd(2)-Cl(3)	2.6140(19)	N(7)-C(5)	1.375(10)	C(10')-C(11')	1.506(11)
Cd(2)-Cl(2)#1	2.6242(19)	N(7)-C(10)	1.476(10)	C(10')-H(10C)	0.9700
Cd(2)-Cl(5)	2.6298(18)	N(7')-C(8')	1.330(11)	C(10')-H(10D)	0.9700
Cd(3)-N(3')	2.390(7)	N(7')-C(5')	1.385(11)	C(11)-C(12)	1.338(13)
Cd(3)-N(3')#2	2.390(7)	N(7')-C(10')	1.476(10)	C(11)-H(11)	0.9300
Cd(3)-Cl(4)#2	2.6219(18)	N(9)-C(8)	1.339(10)	C(11')-C(12')	1.313(15)
Cd(3)-Cl(4)	2.6219(18)	N(9)-C(4)	1.385(10)	C(11')-H(11')	0.9300
Cd(3)-Cl(5)#2	2.6331(19)	N(9')-C(8')	1.320(11)	C(12)-H(12A)	0.9300
Cd(3)-Cl(5)	2.6331(19)	N(9')-C(4')	1.392(10)	C(12)-H(12B)	0.9300
Cl(1)-C(6)	1.724(8)	C(2)-H(2)	0.9300	C(12')-H(12C)	0.9300
Cl(1')-C(6')	1.713(9)	C(2')-H(2')	0.9300	C(12')-H(12D)	0.9300

10.15 Bond angles of CdACP:

N(3)#1-Cd(1)-N(3)	180.0(3)	N(3')#2-Cd(3)-Cl(5)	90.44(17)	N(7)-C(5)-C(4)	105.7(7)
N(3)#1-Cd(1)-Cl(2)	90.42(16)	Cl(4)#2-Cd(3)-Cl(5)	96.30(6)	C(6)-C(5)-C(4)	117.7(7)
N(3)-Cd(1)-Cl(2)	89.58(16)	Cl(4)-Cd(3)-Cl(5)	83.70(6)	C(6')-C(5')-N(7')	136.4(8)
N(3)#1-Cd(1)-Cl(2)#1	89.58(16)	Cl(5)#2-Cd(3)-Cl(5)	180.00(6)	C(6')-C(5')-C(4')	117.9(7)
N(3)-Cd(1)-Cl(2)#1	90.42(16)	Cd(1)-Cl(2)-Cd(2)#1	92.18(6)	N(7')-C(5')-C(4')	105.7(7)
Cl(2)-Cd(1)-Cl(2)#1	180.0	Cd(2)-Cl(3)-Cd(1)	91.10(6)	N(1)-C(6)-C(5)	120.6(8)
N(3)#1-Cd(1)-Cl(3)	89.39(17)	Cd(2)-Cl(4)-Cd(3)	91.50(6)	N(1)-C(6)-Cl(1)	116.7(6)
N(3)-Cd(1)-Cl(3)	90.61(17)	Cd(2)-Cl(5)-Cd(3)	90.85(6)	C(5)-C(6)-Cl(1)	122.6(6)
Cl(2)-Cd(1)-Cl(3)	95.94(6)	C(6)-N(1)-C(2)	116.3(7)	N(1')-C(6')-C(5')	119.3(8)
Cl(2)#1-Cd(1)-Cl(3)	84.06(6)	C(2')-N(1')-C(6')	118.1(7)	N(1')-C(6')-Cl(1')	117.6(7)
N(3)#1-Cd(1)-Cl(3)#1	90.61(17)	C(2)-N(3)-C(4)	114.1(7)	C(5')-C(6')-Cl(1')	123.0(7)
N(3)-Cd(1)-Cl(3)#1	89.39(17)	C(2)-N(3)-Cd(1)	113.8(5)	N(7)-C(8)-N(9)	114.5(7)
Cl(2)-Cd(1)-Cl(3)#1	84.06(6)	C(4)-N(3)-Cd(1)	127.2(6)	N(7)-C(8)-H(8)	122.7
Cl(2)#1-Cd(1)-Cl(3)#1	95.94(6)	C(2')-N(3')-C(4')	113.8(7)	N(9)-C(8)-H(8)	122.7
Cl(3)-Cd(1)-Cl(3)#1	180.0	C(2')-N(3')-Cd(3)	115.1(5)	N(9')-C(8')-N(7')	116.2(7)
N(9')-Cd(2)-N(9)	89.3(2)	C(4')-N(3')-Cd(3)	130.6(5)	N(9')-C(8')-H(8')	121.9
N(9')-Cd(2)-Cl(4)	90.67(17)	C(8)-N(7)-C(5)	106.6(7)	N(7')-C(8')-H(8')	121.9
N(9)-Cd(2)-Cl(4)	171.34(16)	C(8)-N(7)-C(10)	125.2(7)	N(7)-C(10)-C(11)	112.7(7)
N(9')-Cd(2)-Cl(3)	164.97(17)	C(5)-N(7)-C(10)	128.1(7)	N(7)-C(10)-H(10A)	109.1
N(9)-Cd(2)-Cl(3)	82.78(16)	C(8')-N(7')-C(5')	105.4(7)	C(11)-C(10)-H(10A)	109.1
Cl(4)-Cd(2)-Cl(3)	99.11(6)	C(8')-N(7')-C(10')	126.1(7)	N(7)-C(10)-H(10B)	109.1
N(9')-Cd(2)-Cl(2)#1	83.87(17)	C(5')-N(7')-C(10')	128.1(7)	C(11)-C(10)-H(10B)	109.1
N(9)-Cd(2)-Cl(2)#1	93.30(16)	C(8)-N(9)-C(4)	103.3(7)	H(10A)-C(10)-H(10B)	107.8
Cl(4)-Cd(2)-Cl(2)#1	95.31(6)	C(8)-N(9)-Cd(2)	122.8(5)	N(7')-C(10')-C(11')	112.9(7)
Cl(3)-Cd(2)-Cl(2)#1	83.89(6)	C(4)-N(9)-Cd(2)	132.8(5)	N(7')-C(10')-H(10C)	109.0
N(9')-Cd(2)-Cl(5)	88.33(17)	C(8')-N(9')-C(4')	102.7(7)	C(11')-C(10')-H(10C)	109.0
N(9)-Cd(2)-Cl(5)	87.38(16)	C(8')-N(9')-Cd(2)	122.9(5)	N(7')-C(10')-H(10D)	109.0
Cl(4)-Cd(2)-Cl(5)	83.96(6)	C(4')-N(9')-Cd(2)	133.8(5)	C(11')-C(10')-H(10D)	109.0
Cl(3)-Cd(2)-Cl(5)	103.94(6)	N(3)-C(2)-N(1)	129.1(8)	H(10C)-C(10')-H(10D)	107.8
Cl(2)#1-Cd(2)-Cl(5)	172.16(6)	N(3)-C(2)-H(2)	115.5	C(12)-C(11)-C(10)	122.8(8)
N(3')-Cd(3)-N(3')#2	180.0	N(1)-C(2)-H(2)	115.5	C(12)-C(11)-H(11)	118.6
N(3')-Cd(3)-Cl(4)#2	87.56(16)	N(1')-C(2')-N(3')	127.9(8)	C(10)-C(11)-H(11)	118.6

N(3')#2-Cd(3)-Cl(4)#2	92.44(16)	N(1')-C(2')-H(2')	116.1	C(12')-C(11')-C(10')	121.9(10)
N(3')-Cd(3)-Cl(4)	92.44(16)	N(3')-C(2')-H(2')	116.1	C(12')-C(11')-H(11')	119.1
N(3')#2-Cd(3)-Cl(4)	87.56(16	N(3)-C(4)-N(9)	128.0(7)	C(10')-C(11')-H(11')	119.1
Cl(4)#2-Cd(3)-Cl(4)	180.0	N(3)-C(4)-C(5)	122.1(7)	C(11)-C(12)-H(12A)	120.0
N(3')-Cd(3)-Cl(5)#2	90.44(17)	N(9)-C(4)-C(5)	109.8(7)	C(11)-C(12)-H(12B)	120.0
N(3')#2-Cd(3)-Cl(5)#2	89.56(17)	N(3')-C(4')-N(9')	127.1(7)	H(12A)-C(12)-H(12B)	120.0
Cl(4)#2-Cd(3)-Cl(5)#2	83.70(6)	N(3')-C(4')-C(5')	122.9(7)	C(11')-C(12')-H(12C)	120.0
Cl(4)-Cd(3)-Cl(5)#2	96.30(6)	N(9')-C(4')-C(5')	109.9(7)	C(11')-C(12')-H(12D)	120.0
N(3')-Cd(3)-Cl(5)	89.56(17)	N(7)-C(5)-C(6)	136.6(8)	H(12C)-C(12')-H(12D)	120.0

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z+1 #2 -x,-y+1,-z+2

10.16 Hydrogen bond table for CdBCP:

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(8)-H(8)...O(1)	0.95	2.23	3.134(13)	159.5
C(2)-H(2)...Cl(2)	0.95	2.94	3.511(8)	120.1
C(2')-H(2')...Cl(2)#3	0.95	2.95	3.852(9)	159.7
C(10)-H(10B)...Cl(2)#4	0.99	2.73	3.701(9)	168.6
C(10')-H(10D)...Cl(4)#5	0.99	2.69	3.664(8)	169.1

Symmetry transformations used to generate equivalent atoms:

#1 x+1/2,-y+2,z #2 x-1/2,-y+2,z #3 x-1,y,z

#4 x+0,-y+3/2,z+1/2 #5 x-1/2,y-1/2,z-1/2

10.17 Bond length of CdBCP

	Bond lengths [Å]		Bond lengths [Å]		Bond lengths [Å]
Cd(1)-N(3)	2.396(6)	N(7)-C(10)	1.482(9)	C(11')-C(12')	1.390(12)
Cd(1)-N(3')#1	2.421(6)	N(7')-C(8')	1.358(11)	C(11')-C(16')	1.392(13)
Cd(1)-Cl(2)	2.567(2)	N(7')-C(5')	1.401(12)	C(12)-C(13)	1.396(13)
Cd(1)-Cl(4)	2.588(2)	N(7')-C(10')	1.458(10)	C(12)-H(12)	0.9500
Cd(1)-Cl(3)	2.6204(19)	N(9)-C(8)	1.324(11)	C(12')-C(13')	1.360(15)
Cd(1)-Cl(5)#1	2.6292(19)	N(9)-C(4)	1.380(11)	C(12')-H(12')	0.9500
Cd(2)-N(9)	2.358(6)	N(9')-C(8')	1.312(10)	C(13)-C(14)	1.400(13)
Cd(2)-N(9')	2.384(7)	N(9')-C(4')	1.381(11)	C(13)-H(13)	0.9500
Cd(2)-Cl(4)	2.5638(18)	C(2)-H(2)	0.9500	C(13')-C(14')	1.401(18)
Cd(2)-Cl(2)#2	2.6052(18)	C(2')-H(2')	0.9500	C(13')-H(13')	0.9500
Cd(2)-Cl(3)	2.620(2)	C(4)-C(5)	1.407(10)	C(14)-C(15)	1.363(13)
Cd(2)-Cl(5)	2.624(2)	C(4')-C(5')	1.385(10)	C(14)-H(14)	0.9500
Cl(1)-C(6)	1.732(8)	C(5)-C(6)	1.371(12)	C(14')-C(15')	1.394(15)
Cl(1')-C(6')	1.713(7)	C(5')-C(6')	1.406(12)	C(14')-H(14')	0.9500
N(1)-C(6)	1.318(11)	C(8)-H(8)	0.9500	C(15)-C(16)	1.382(12)
N(1)-C(2)	1.352(10)	C(8')-H(8')	0.9500	C(15)-H(15)	0.9500
N(1')-C(6')	1.312(11)	C(10)-C(11)	1.514(11)	C(15')-C(16')	1.391(13)
N(1')-C(2')	1.357(10)	C(10)-H(10A)	0.9900	C(15')-H(15')	0.9500

N(3)-C(2)	1.325(11)	C(10)-H(10B)	0.9900	C(16)-H(16)	0.9500
N(3)-C(4)	1.360(10)	C(10')-C(11')	1.512(11)	C(16')-H(16')	0.9500
N(3')-C(4')	1.326(11)	C(10')-H(10C)	0.9900	O(1)-H(1A)	0.8501
N(3')-C(2')	1.331(11)	C(10')-H(10D)	0.9900	O(1)-H(1B)	0.8501
N(7)-C(8)	1.348(11)	C(11)-C(12)	1.375(11)		
N(7)-C(5)	1.372(12)	C(11)-C(16)	1.408(11)		

10.18 Bond angles of CdBCP:

	angles [°]		angles [°]		angles [°]
N(3)-Cd(1)-N(3')#1	177.6(3)	C(8')-N(7')-C(5')	104.4(7)	N(7')-C(10')-C(11')	114.4(7)
N(3)-Cd(1)-Cl(2)	89.71(17)	C(8')-N(7')-C(10')	126.0(8)	N(7')-C(10')-H(10C)	108.6
N(3')#1-Cd(1)-Cl(2)	90.32(18)	C(5')-N(7')-C(10')	129.6(7)	C(11')-C(10')-H(10C)	108.6
N(3)-Cd(1)-Cl(4)	91.92(17)	C(8)-N(9)-C(4)	103.5(7)	N(7')-C(10')-H(10D)	108.7
N(3')#1-Cd(1)-Cl(4)	88.15(18)	C(8)-N(9)-Cd(2)	123.6(6)	C(11')-C(10')-H(10D)	108.6
Cl(2)-Cd(1)-Cl(4)	176.91(7)	C(4)-N(9)-Cd(2)	132.8(5)	H(10C)-C(10')-H(10D)	107.6
N(3)-Cd(1)-Cl(3)	87.65(16)	C(8')-N(9')-C(4')	104.8(7)	C(12)-C(11)-C(16)	119.1(8)
N(3')#1-Cd(1)-Cl(3)	89.98(16)	C(8')-N(9')-Cd(2)	121.7(6)	C(12)-C(11)-C(10)	119.5(8)
Cl(2)-Cd(1)-Cl(3)	93.11(6)	C(4')-N(9')-Cd(2)	133.5(5)	C(16)-C(11)-C(10)	121.0(7)
Cl(4)-Cd(1)-Cl(3)	89.58(6)	N(3)-C(2)-N(1)	127.2(8)	C(12')-C(11')-C(16')	119.8(8)
N(3)-Cd(1)-Cl(5)#1	92.54(16)	N(3)-C(2)-H(2)	116.4	C(12')-C(11')-C(10')	117.5(8)
N(3')#1-Cd(1)-Cl(5)#1	89.83(16)	N(1)-C(2)-H(2)	116.4	C(16')-C(11')-C(10')	122.6(7)
Cl(2)-Cd(1)-Cl(5)#1	89.60(6)	N(3')-C(2')-N(1')	126.8(8)	C(11)-C(12)-C(13)	120.2(8)
Cl(4)-Cd(1)-Cl(5)#1	87.71(6)	N(3')-C(2')-H(2')	116.6	C(11)-C(12)-H(12)	119.9
Cl(3)-Cd(1)-Cl(5)#1	177.29(8)	N(1')-C(2')-H(2')	116.6	C(13)-C(12)-H(12)	119.9
N(9)-Cd(2)-N(9')	91.32(17)	N(3)-C(4)-N(9)	126.9(7)	C(13')-C(12')-C(11')	120.5(10)
N(9)-Cd(2)-Cl(4)	88.51(17)	N(3)-C(4)-C(5)	122.9(8)	C(13')-C(12')-H(12')	119.8
N(9')-Cd(2)-Cl(4)	176.94(17)	N(9)-C(4)-C(5)	110.2(7)	C(11')-C(12')-H(12')	119.8
N(9)-Cd(2)-Cl(2)#2	177.79(19)	N(3')-C(4')-N(9')	126.8(7)	C(12)-C(13)-C(14)	120.3(8)
N(9')-Cd(2)-Cl(2)#2	87.84(16)	N(3')-C(4')-C(5')	123.7(8)	C(12)-C(13)-H(13)	119.8
Cl(4)-Cd(2)-Cl(2)#2	92.44(5)	N(9')-C(4')-C(5')	109.5(7)	C(14)-C(13)-H(13)	119.8
N(9)-Cd(2)-Cl(3)	87.80(18)	C(6)-C(5)-N(7)	137.3(7)	C(12')-C(13')-C(14')	121.0(9)
N(9')-Cd(2)-Cl(3)	86.83(17)	C(6)-C(5)-C(4)	117.3(8)	C(12')-C(13')-H(13')	119.5
Cl(4)-Cd(2)-Cl(3)	90.11(6)	N(7)-C(5)-C(4)	105.3(7)	C(14')-C(13')-H(13')	119.5
Cl(2)#2-Cd(2)-Cl(3)	94.19(6)	C(4')-C(5')-N(7')	106.6(7)	C(15)-C(14)-C(13)	119.0(8)
N(9)-Cd(2)-Cl(5)	89.04(18)	C(4')-C(5')-C(6')	117.4(8)	C(15)-C(14)-H(14)	120.5
N(9')-Cd(2)-Cl(5)	87.89(17)	N(7')-C(5')-C(6')	135.9(7)	C(13)-C(14)-H(14)	120.5

Cl(4)-Cd(2)-Cl(5)	95.16(6)	N(1)-C(6)-C(5)	120.8(7)	C(15')-C(14')-C(13')	118.4(9)
Cl(2)#2-Cd(2)-Cl(5)	88.89(6)	N(1)-C(6)-Cl(1)	116.4(7)	C(15')-C(14')-H(14')	120.8
Cl(3)-Cd(2)-Cl(5)	173.79(5)	C(5)-C(6)-Cl(1)	122.7(7)	C(13')-C(14')-H(14')	120.8
Cd(1)-Cl(2)-Cd(2)#1	88.69(6)	N(1')-C(6')-C(5')	119.6(7)	C(14)-C(15)-C(16)	121.4(8)
Cd(2)-Cl(3)-Cd(1)	86.52(5)	N(1')-C(6')-Cl(1')	118.2(6)	C(14)-C(15)-H(15)	119.3
Cd(2)-Cl(4)-Cd(1)	88.40(6)	C(5')-C(6')-Cl(1')	122.2(6)	C(16)-C(15)-H(15)	119.3
Cd(2)-Cl(5)-Cd(1)#2	86.97(5)	N(9)-C(8)-N(7)	114.5(8)	C(16')-C(15')-C(14')	120.8(10)
C(6)-N(1)-C(2)	118.1(7)	N(9)-C(8)-H(8)	122.7	C(16')-C(15')-H(15')	119.6
C(6')-N(1')-C(2')	118.1(7)	N(7)-C(8)-H(8)	122.7	C(14')-C(15')-H(15')	119.6
C(2)-N(3)-C(4)	113.7(7)	N(9')-C(8')-N(7')	114.6(8)	C(15)-C(16)-C(11)	119.9(8)
C(2)-N(3)-Cd(1)	118.4(5)	N(9')-C(8')-H(8')	122.7	C(15)-C(16)-H(16)	120.1
C(4)-N(3)-Cd(1)	127.9(5)	N(7')-C(8')-H(8')	122.7	C(11)-C(16)-H(16)	120.1
C(4')-N(3')-C(2')	114.4(7)	N(7)-C(10)-C(11)	112.1(7)	C(15')-C(16')-C(11')	119.4(9)
C(4')-N(3')-Cd(1)#2	128.6(5)	N(7)-C(10)-H(10A)	109.2	C(15')-C(16')-H(16')	120.3
C(2')-N(3')-Cd(1)#2	117.0(5)	C(11)-C(10)-H(10A)	109.2	C(11')-C(16')-H(16')	120.3
C(8)-N(7)-C(5)	106.4(6)	N(7)-C(10)-H(10B)	109.2	H(1A)-O(1)-H(1B)	109.5
C(8)-N(7)-C(10)	123.5(8)	C(11)-C(10)-H(10B)	109.2		
C(5)-N(7)-C(10)	130.1(7)	H(10A)-C(10)-H(10B)	107.9		

10.19 Hydrogen bond table for HgMCP

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(8)-H(8)...Cl(1)#4	0.93	2.90	3.806(8)	163.9
C(10)-H(10A)...N(1)#4	0.96	2.63	3.558(10)	161.7
C(10)-H(10B)...Cl(2)#5	0.96	2.78	3.591(8)	142.1
C(10)-H(10C)...Cl(2)#6	0.96	2.87	3.523(9)	126.2

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z+1 #2 -x+1,y,-z+1/2 #3 x,-y,z+1/2

#4 x,-y+1,z-1/2 #5 -x+1,-y+1,-z+1 #6 x-1/2,-y+1/2,-z+1

10.20 Bond lengths of HgMCP:

	Bond lengths [Å]		Bond lengths [Å]		Bond lengths [Å]
Hg(1)-Cl(2)	2.3561(18)	Hg(2)-N(9)#2	2.572(7)	N(9)-C(8)	1.309(11)
Hg(1)-Cl(2)#1	2.3562(18)	Cl(1)-C(6)	1.803(9)	N(9)-C(4)	1.389(9)
Hg(1)-N(3)#1	2.677(7)	N(1)-C(6)	1.325(11)	C(2)-H(2)	0.9300
Hg(1)-N(3)	2.677(7)	N(1)-C(2)	1.340(11)	C(4)-C(5)	1.383(12)
Hg(1)-Cl(3)#2	2.9712(18)	N(3)-C(2)	1.330(10)	C(5)-C(6)	1.381(11)
Hg(1)-Cl(3)#3	2.9712(18)	N(3)-C(4)	1.338(10)	C(8)-H(8)	0.9300
Hg(2)-Cl(3)#2	2.3594(18)	N(7)-C(8)	1.348(10)	C(10)-H(10A)	0.9600
Hg(2)-Cl(3)	2.3594(18)	N(7)-C(5)	1.384(10)	C(10)-H(10B)	0.9600
Hg(2)-N(9)	2.572(7)	N(7)-C(10)	1.458(10)	C(10)-H(10C)	0.9600

10.21 Bond angles of HgMCP:

	angles [°]		angles [°]		angles [°]
Cl(2)-Hg(1)-Cl(2)#1	180.0	Cl(3)#2-Hg(2)-N(9)#2	94.88(16)	N(3)-C(4)-N(9)	125.9(7)
Cl(2)-Hg(1)-N(3)#1	91.21(15)	Cl(3)-Hg(2)-N(9)#2	98.95(15)	C(5)-C(4)-N(9)	110.2(7)
Cl(2)#1-Hg(1)-N(3)#1	88.79(15)	N(9)-Hg(2)-N(9)#2	83.6(3)	C(6)-C(5)-C(4)	117.4(7)
Cl(2)-Hg(1)-N(3)	88.79(15)	Hg(2)-Cl(3)-Hg(1)#2	92.80(6)	C(6)-C(5)-N(7)	136.8(8)
Cl(2)#1-Hg(1)-N(3)	91.21(15)	C(6)-N(1)-C(2)	117.6(7)	C(4)-C(5)-N(7)	105.8(7)
N(3)#1-Hg(1)-N(3)	180.0(3)	C(2)-N(3)-C(4)	113.6(7)	N(1)-C(6)-C(5)	120.2(8)
Cl(2)-Hg(1)-Cl(3)#2	93.08(6)	C(2)-N(3)-Hg(1)	114.2(5)	N(1)-C(6)-Cl(1)	117.2(6)
Cl(2)#1-Hg(1)-Cl(3)#2	86.92(6)	C(4)-N(3)-Hg(1)	132.0(5)	C(5)-C(6)-Cl(1)	122.6(7)
N(3)#1-Hg(1)-Cl(3)#2	91.34(15)	C(8)-N(7)-C(5)	105.4(7)	N(9)-C(8)-N(7)	115.0(7)
N(3)-Hg(1)-Cl(3)#2	88.66(15)	C(8)-N(7)-C(10)	126.5(7)	N(9)-C(8)-H(8)	122.5
Cl(2)-Hg(1)-Cl(3)#3	86.92(6)	C(5)-N(7)-C(10)	128.1(7)	N(7)-C(8)-H(8)	122.5
Cl(2)#1-Hg(1)-Cl(3)#3	93.08(6)	C(8)-N(9)-C(4)	103.5(7)	N(7)-C(10)-H(10A)	109.5
N(3)#1-Hg(1)-Cl(3)#3	88.66(15)	C(8)-N(9)-Hg(2)	121.7(5)	N(7)-C(10)-H(10B)	109.5
N(3)-Hg(1)-Cl(3)#3	91.34(15)	C(4)-N(9)-Hg(2)	132.9(5)	H(10A)-C(10)-H(10B)	109.5
Cl(3)#2-Hg(1)-Cl(3)#3	180.0	N(3)-C(2)-N(1)	127.4(7)	N(7)-C(10)-H(10C)	109.5
Cl(3)#2-Hg(2)-Cl(3)	161.41(11)	N(3)-C(2)-H(2)	116.3	H(10A)-C(10)-H(10C)	109.5
Cl(3)#2-Hg(2)-N(9)	98.95(15)	N(1)-C(2)-H(2)	116.3	H(10B)-C(10)-H(10C)	109.5
Cl(3)-Hg(2)-N(9)	94.88(16)	N(3)-C(4)-C(5)	123.8(7)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z+1 #2 -x+1,y,-z+1/2 #3 x,-y,z+1/2

10.22 Hydrogen bond table for HgACP

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(8)-H(8)...N(1)#3	0.95	2.37	3.294(15)	164.9
C(10)-H(10A)...Cl(1)	0.99	2.88	3.407(16)	113.8
C(10)-H(10A)...Cl(2)#4	0.99	2.74	3.337(13)	119.2

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z+1 #2 -x+1,y,-z+3/2 #3 x,-y+1,z+1/2

#4 -x+1,-y+1,-z+1

10.23 Bond length of HgACP

	Bond lengths [Å]		Bond lengths [Å]		Bond lengths [Å]
Hg(1)-Cl(2)	2.336(3)	N(1)-C(2)	1.372(15)	C(5)-C(6)	1.395(15)
Hg(1)-Cl(2)#1	2.336(3)	N(3)-C(2)	1.330(13)	C(8)-H(8)	0.9500
Hg(1)-N(3)	2.649(10)	N(3)-C(4)	1.354(14)	C(10)-C(11)	1.42(2)
Hg(1)-N(3)#1	2.649(10)	N(7)-C(5)	1.380(14)	C(10)-H(10A)	0.9900
Hg(2)-Cl(3)#2	2.369(2)	N(7)-C(8)	1.390(16)	C(10)-H(10B)	0.9900
Hg(2)-Cl(3)	2.369(2)	N(7)-C(10)	1.474(16)	C(11)-C(12)	1.35(2)
Hg(2)-N(9)	2.499(10)	N(9)-C(8)	1.316(15)	C(11)-H(11)	0.9500
Hg(2)-N(9)#2	2.499(10)	N(9)-C(4)	1.394(13)	C(12)-H(12A)	0.9500
Cl(1)-C(6)	1.731(13)	C(2)-H(2)	0.9500	C(12)-H(12B)	0.9500
N(1)-C(6)	1.307(16)	C(4)-C(5)	1.354(15)		

10.24 Bond angle of HgACP

	angles [°]		angles [°]		angles [°]
Cl(2)-Hg(1)-Cl(2)#1	180.0	C(5)-N(7)-C(10)	131.6(11)	N(9)-C(8)-N(7)	113.3(10)
Cl(2)-Hg(1)-N(3)	89.3(2)	C(8)-N(7)-C(10)	123.0(11)	N(9)-C(8)-H(8)	123.4
Cl(2)#1-Hg(1)-N(3)	90.7(2)	C(8)-N(9)-C(4)	103.7(10)	N(7)-C(8)-H(8)	123.4
Cl(2)-Hg(1)-N(3)#1	90.7(2)	C(8)-N(9)-Hg(2)	120.0(8)	C(11)-C(10)-N(7)	113.3(13)
Cl(2)#1-Hg(1)-N(3)#1	89.3(2)	C(4)-N(9)-Hg(2)	134.5(7)	C(11)-C(10)-H(10A)	108.9
N(3)-Hg(1)-N(3)#1	180.0	N(3)-C(2)-N(1)	128.6(11)	N(7)-C(10)-H(10A)	108.9

Cl(3)#2-Hg(2)-Cl(3)	159.10(16)	N(3)-C(2)-H(2)	115.7	C(11)-C(10)-H(10B)	108.9
Cl(3)#2-Hg(2)-N(9)	91.4(2)	N(1)-C(2)-H(2)	115.7	N(7)-C(10)-H(10B)	108.9
Cl(3)-Hg(2)-N(9)	103.7(2)	N(3)-C(4)-C(5)	125.5(10)	H(10A)-C(10)-H(10B)	107.7
Cl(3)#2-Hg(2)-N(9)#2	103.7(2)	N(3)-C(4)-N(9)	123.2(10)	C(12)-C(11)-C(10)	122.4(16)
Cl(3)-Hg(2)-N(9)#2	91.4(2)	C(5)-C(4)-N(9)	111.2(10)	C(12)-C(11)-H(11)	118.8
N(9)-Hg(2)-N(9)#2	88.3(5)	C(4)-C(5)-N(7)	107.0(9)	C(10)-C(11)-H(11)	118.8
C(6)-N(1)-C(2)	116.1(10)	C(4)-C(5)-C(6)	117.0(11)	C(11)-C(12)-H(12A)	120.0
C(2)-N(3)-C(4)	111.4(10)	N(7)-C(5)-C(6)	135.9(11)	C(11)-C(12)-H(12B)	120.0
C(2)-N(3)-Hg(1)	109.1(7)	N(1)-C(6)-C(5)	121.0(12)	H(12A)-C(12)-H(12B)	120.0
C(4)-N(3)-Hg(1)	129.2(7)	N(1)-C(6)-Cl(1)	116.8(9)		
C(5)-N(7)-C(8)	104.9(9)	C(5)-C(6)-Cl(1)	122.2(10)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z+1 #2 -x+1,y,-z+3/2

10.25 Hydrogen bond table for HgBCP

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(8)-H(8)...Cl(3)#1	0.93	2.80	3.323(7)	116.3
C(8)-H(8)...Cl(4)#2	0.93	2.90	3.779(8)	157.3
C(10)-H(10B)...Cl(1)	0.97	2.89	3.426(9)	116.0

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1 #2 x,-y+3/2,z-1/2

10.26 Bond length of HgBCP

	Bond lengths [Å]		Bond lengths [Å]		Bond lengths [Å]
Hg(1)-Cl(2)	2.308(2)	N(2)-C(2)	1.324(11)	C(11)-C(16)	1.384(11)
Hg(1)-Cl(3)	2.352(2)	N(3)-C(8)	1.341(9)	C(11)-C(12)	1.400(10)
Hg(1)-Cl(4)	2.738(2)	N(3)-C(5)	1.391(10)	C(12)-C(13)	1.392(13)
Hg(2)-N(4)	2.226(6)	N(3)-C(10)	1.479(10)	C(12)-H(12)	0.9300
Hg(2)-N(4)#1	2.226(6)	N(4)-C(8)	1.325(10)	C(13)-C(14)	1.379(14)
Hg(2)-Cl(4)	2.779(2)	N(4)-C(4)	1.381(10)	C(13)-H(13)	0.9300
Hg(2)-Cl(4)#1	2.779(2)	C(2)-H(2)	0.9300	C(14)-C(15)	1.373(13)
Hg(2)-Cl(3)	2.799(2)	C(4)-C(5)	1.409(10)	C(14)-H(14)	0.9300
Hg(2)-Cl(3)#1	2.799(2)	C(5)-C(6)	1.390(11)	C(15)-C(16)	1.377(12)
Cl(1)-C(6)	1.740(8)	C(8)-H(8)	0.9300	C(15)-H(15)	0.9300
N(1)-C(6)	1.304(12)	C(10)-C(11)	1.505(10)	C(16)-H(16)	0.9300
N(1)-C(2)	1.333(12)	C(10)-H(10A)	0.9700		
N(2)-C(4)	1.324(10)	C(10)-H(10B)	0.9700		

10.27 Bond angle of HgBCP

	angles [°]		angles [°]		angles [°]
Cl(2)-Hg(1)-Cl(3)	157.79(9)	C(8)-N(3)-C(5)	105.7(6)	N(3)-C(10)-H(10A)	108.9
Cl(2)-Hg(1)-Cl(4)	107.96(9)	C(8)-N(3)-C(10)	124.1(7)	C(11)-C(10)-H(10A)	108.9
Cl(3)-Hg(1)-Cl(4)	94.15(7)	C(5)-N(3)-C(10)	130.2(6)	N(3)-C(10)-H(10B)	108.9
N(4)-Hg(2)-N(4)#1	180.0	C(8)-N(4)-C(4)	105.4(6)	C(11)-C(10)-H(10B)	108.9
N(4)-Hg(2)-Cl(4)	92.97(17)	C(8)-N(4)-Hg(2)	123.0(5)	H(10A)-C(10)-H(10B)	107.7
N(4)#1-Hg(2)-Cl(4)	87.03(17)	C(4)-N(4)-Hg(2)	131.1(5)	C(16)-C(11)-C(12)	118.5(7)
N(4)-Hg(2)-Cl(4)#1	87.03(17)	N(2)-C(2)-N(1)	127.5(8)	C(16)-C(11)-C(10)	121.7(7)
N(4)#1-Hg(2)-Cl(4)#1	92.97(17)	N(2)-C(2)-H(2)	116.2	C(12)-C(11)-C(10)	119.7(7)
Cl(4)-Hg(2)-Cl(4)#1	180.0	N(1)-C(2)-H(2)	116.2	C(13)-C(12)-C(11)	120.3(8)
N(4)-Hg(2)-Cl(3)	96.62(19)	N(2)-C(4)-N(4)	127.5(7)	C(13)-C(12)-H(12)	119.8
N(4)#1-Hg(2)-Cl(3)	83.38(19)	N(2)-C(4)-C(5)	124.1(7)	C(11)-C(12)-H(12)	119.8

Cl(4)-Hg(2)-Cl(3)	84.11(6)	N(4)-C(4)-C(5)	108.4(6)	C(14)-C(13)-C(12)	119.7(8)
Cl(4)#1-Hg(2)-Cl(3)	95.89(6)	C(6)-C(5)-N(3)	138.4(7)	C(14)-C(13)-H(13)	120.2
N(4)-Hg(2)-Cl(3)#1	83.38(19)	C(6)-C(5)-C(4)	115.2(7)	C(12)-C(13)-H(13)	120.2
N(4)#1-Hg(2)-Cl(3)#1	96.62(19)	N(3)-C(5)-C(4)	106.4(6)	C(15)-C(14)-C(13)	120.1(8)
Cl(4)-Hg(2)-Cl(3)#1	95.89(6)	N(1)-C(6)-C(5)	121.4(8)	C(15)-C(14)-H(14)	119.9
Cl(4)#1-Hg(2)-Cl(3)#1	84.11(6)	N(1)-C(6)-Cl(1)	117.1(6)	C(13)-C(14)-H(14)	119.9
Cl(3)-Hg(2)-Cl(3)#1	180.0	C(5)-C(6)-Cl(1)	121.4(7)	C(14)-C(15)-C(16)	120.5(8)
Hg(1)-Cl(3)-Hg(2)	90.28(7)	N(4)-C(8)-N(3)	114.1(7)	C(14)-C(15)-H(15)	119.7
Hg(1)-Cl(4)-Hg(2)	83.23(6)	N(4)-C(8)-H(8)	123.0	C(16)-C(15)-H(15)	119.7
C(6)-N(1)-C(2)	117.8(7)	N(3)-C(8)-H(8)	123.0	C(15)-C(16)-C(11)	120.8(8)
C(4)-N(2)-C(2)	113.8(7)	N(3)-C(10)-C(11)	113.3(7)	C(15)-C(16)-H(16)	119.6

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1

11 Reference:

[1] O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard, H. Puschmann, *J. Appl. Crystallogr.* **2009**, *42*, 339-341.

[2] G. Sheldrick, *Acta Crystallographica Section A* **2015**, *71*, 3-8.

[3] G. Sheldrick, *Acta Crystallographica Section C* **2015**, *71*, 3-8.

[4] S. Chen, R. F. Graceffa, A. A. Boezio, *Org. Lett.* **2016**, *18*, 16-19.

[5] H. E. Gottlieb, V. Kotlyar, A. Nudelman, *The Journal of Organic Chemistry* **1997**, *62*, 7512-7515.

[6] E. L. Unger, E. T. Hoke, C. D. Bailie, W. H. Nguyen, A. R. Bowring, T. Heumüller, M. G. Christoforo, M. D. McGehee, *Energy & Environmental Science* **2014**, *7*, 3690-3698.

[7] Y.-C. Zhao, W.-K. Zhou, X. Zhou, K.-H. Liu, D.-P. Yu, Q. Zhao, *Light: Science & Applications* **2017**, *6*, e16243-e16243.

[8] V. K. Sangwan, H.-S. Lee, H. Bergeron, I. Balla, M. E. Beck, K.-S. Chen, M. C. Hersam, *Nature* **2018**, *554*, 500-504.