Self-assembly of metal-organic hybrid nanoscopic rectangles

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Table S1 - Crystal Data and Details of the Structure Determination
for: rectangle-1 C 2/c R = 0.08

Crystal Data

Formula	C_{98} H_{15}4 N_{10} O_{14} P_8 Pt_4
Formula Weight	2724.43
Crystal System	Monoclinic
Space group	C2/c (No. 15)
a, b, c [Angstrom]	40.6123(13) 14.7952(4) 20.0041(7)
alpha, beta, gamma [deg]	90, 98.1700(10) ,90
V [Ang**3]	11897.8(7)
Z	4
D(calc) [g/cm**3]	1.521
Mu(MoKa) [/mm]	4.853
F(000)	5424
Crystal Size [mm]	0.13 x 0.28 x 0.38
Temperature (K)	150
Radiation [Angstrom]	MoKa 0.71073
Theta Min-Max [Deg]	1.8, 27.4
Tot., Uniq. Data, R(int)	25167, 13441, 0.069
Observed data [I > 2.0 sigma(I)]	7163
Nref, Npar	13441, 513
R, wR2, S	0.0823, 0.2427, 1.11
w = 1/[\S^2^(FO^2^)+(0.1003P)^2^+136.1806P] WHERE P=(FO^2^+2FC^2^)	
Min. and Max. Resd. Dens. [e/Ang^3]	-2.49, 3.19.

Table **3**. Bond lengths [Å] and angles [°] for **1**.

Pt1-P1	2.320(4)	O2-N4	1.24(3)
Pt1-P2	2.305(4)	O3-N4	1.30(3)
Pt1-N1	2.114(11)	O4-N4	1.17(3)
Pt1-C1	2.027(13)	O8-N6	1.23(3)
Pt2-P3	2.333(4)	O9-N6	1.31(3)
Pt2-P4	2.320(4)	O10-N6	1.38(4)
Pt2-C11	2.009(13)	N1-C19	1.312(16)
Pt2-N3_a	2.132(12)	N1-C15	1.346(18)
P1-C27	1.93(2)	N2-N2A	0.93(3)
P1-C29	1.810(13)	N2-C20	1.35(4)
P1-C31	1.84(2)	N2-C20A	0.77(4)
P2-C33	1.807(14)	N2-C17	1.47(2)
P2-C35	1.89(2)	N2A-C23	1.71(3)
P2-C37	1.855(19)	N2A-C23A	1.45(2)
P3-C45	1.778(14)	N2A-C20	1.28(3)
P3-C47	1.783(17)	N2A-C20A	1.35(3)
P3-C49	1.87(2)	N3-C21	1.35(2)
P4-C39	1.847(17)	N3-C25A	1.34(2)
P4-C41	1.854(13)	N3-C21A	1.32(3)
P4-C43	1.84(2)	N3-C25	1.31(3)
O1-O1A	0.63(3)	N3A-C21	1.35(2)

O1-C20	1.24(3)	N3A-C21A	1.32(3)
O1-C20A	1.47(3)	N3A-C25	1.31(3)
O1A-C20	1.13(3)	N3A-C25A	1.34(2)
O1A-C20A	1.24(3)	N2-H2A1	1.2100
O5-N5	1.28(3)	N2-H2A	0.8800
O6-N5_b	1.35(2)	N2A-H2A1	0.8800
O6-N5	1.35(2)	N2A-H2A	0.8500

P1 -Pt1 -P2	170.13(15)	C45-P3-C49	102.8(8)
P1 -Pt1-N1	90.7(3)	C47-P3 -C49	105.5(8)
P1-Pti-C1	88.6(4)	Pt2-P4-C39	111.8(6)
P2 -Pt1-N1	90.5(3)	Pt2-P4-C41	113.2(5)
P2 -Pt1-C1	90.2(4)	Pt2-P4-C43	112.8(6)
N1-Pt1-C1	179.3(4)	C39-P4 -C41	101.5(8)
P3 -Pt2-P4	169.20(15)	C39-P4-C43	109.5(9)
P3-Pt2-C11	88.3(4)	C41-P4 -C43	107.4(7)
P3-Pt2-N3_a	93.1(3)	O1A -O1 -C20	65(3)
P4 -Pt2-C11	88.6(4)	O1A-O1 -C20A	56(2)
P4-Pt2-N3_a	90.8(3)	C20-O1 -C20A	37.7(18)
N3_a -Pt2 -C11	176.0(6)	O1-O1A -C20	84(3)
Pt1-P1-C27	112.7(7)	O1-O1A-C20A	98(3)
Pt1-P1-C29	116.9(5)	C20 -O1A-C20A	45(2)
Pt1-P1-C31	109.5(6)	N5 -O6-N5_b	180.00
C27-P1 -C29	105.3(8)	Pt1-N1-C19	121.8(9)

C27-P1-C31	105.9(10)	C15-N1-C19	116.8(11)
C29-P1-C31	105.7(8)	Pt1-N1 -C15	121.2(8)
Pt1-P2-C33	114.6(5)	N2A-N2-C17	168(2)
Pt1-P2-C35	110.3(6)	N2A-N2-C20A	105(3)
Pt1-P2-C37	112.4(6)	C17-N2 -C20	120(2)
C33-P2 -C35	108.7(9)	N2A -N2 -C20	65(2)
C33-P2 -C37	102.8(8)	C20-N2-C20A	40(2)
C35-P2 -C37	107.8(8)	C17-N2 -C20A	82(3)
Pt2-P3-C45	113.0(6)	N2-N2A-C20	74(2)
Pt2-P3 -C47	113.0(6)	N2-N2A-C20A	33.7(19)
Pt2-P3-C49	116.1(6)	N2-N2A-C23A	158(2)
C45-P3-C47	105.3(8)	C20-N2A-C20A	40.1(18)
N2-N2A-C23	131(2)	N2-N2A-H2A	59.00
C20-N2A-C23A	85.2(19)	C20-N2A-H2A	131.00
C20A-N2A-C23	97.3(17)	C20A-N2A -H2A1	118.00
C20A-N2A -C23A	124.5(18)	C20-N2A-H2A1	156.00
C23-N2A-C23A	27.3(12)	C23A-N2A-H2A1	118.00
C20-N2A-C23	57.9(18)	C23A-N2A-H2A	139.00
C21 -N3 -C21A	15.3(19)	H2A1 -N2A -H2A	32.00
C21 -N3 -C25A	130.7(19)	C23 -N2A -H2A	161.00
C21A -N3 -C25	103.6(19)	C20A -N2A -H2A	92.00
C21 -N3 -C25	114.6(19)	C23 -N2A -H2A1	145.00
C25 -N3 -C25A	17.9(16)	O5 -N5 -O6	126.8(19)

C21A -N3 -C25A 117.9(19) O3 -N4 -O4 112.8(19)

C21 -N3A -C21A 15.3(19) O2 -N4 -O3 124(2)

C21 -N3A -C25 114.6(19) O2 -N4 -O4 121(2)

C21A -N3A -C25 103.6(19) O8 -N6 -O10 133(2)

C21A -N3A -C25A 117.9(19) O8 -N6 -O9 125(2)

C21 -N3A -C25A 130.7(19) O9 -N6 -O10 96(2)

C17 -N2 -H2A1 126.00 C2 -C1 -C14 117.5(13)

C17 -N2 -H2A 120.00 C1 -C2 -C3 122.3(15)

C20 -N2 -H2A1 111.00 C2 -C3 -C4 119.0(16)

C20 -N2 -H2A 120.00 C3 -C4 -C5 121.7(14)

C20A -N2 -H2A1 150.00 C6 -C5 -C14 118.8(14)

N2A -N2 -H2A1 46.00 C4 -C5 -C14 120.3(15)

H2A1 -N2 -H2A 20.00 C4 -C5 -C6 120.9(13)

C20A -N2 -H2A 155.00 C5 -C6 -C7 123.0(14)

N2 -N2A -H2A1 84.00 C8 -C7 -C12 118.0(15)

C22A -C23A -C24 114(3) C24 -C25A -C24A 24.4(13)

C22A -C23A -C24A 122.0(18) N3 -C25A -C24A 124.6(18)

C23 -C24 -C23A 26(2) N3 -C25A -C24 101.7(16)

C23A -C24 -C25A 139(3) N3 -C25A -C25 77(5)

C24A -C24 -C25 61(2) N3A -C25A -C24 101.7(16)

C23A -C24 -C25 136(3) N3A -C25A -C24A 124.6(18)

C25 -C24 -C25A 9.4(13) C24 -C25A -C25 33(5)

C23 -C24 -C25A 126(2) C24A -C25A -C25 56(5)

C23 -C24 -C24A 160(3) P1 -C27 -C26 118.8(19)

C23 -C24 -C25 119(2) P1 -C29 -C28 122.1(16)

C23A -C24 -C24A 139(4) P1 -C31 -C30 110.2(12)

C24A -C24 -C25A 52(2) P2 -C33 -C32 120.0(12)

C23A -C24A -C25 100.2(19) P2 -C35 -C34 117.3(16)

C23A -C24A -C24 21(2) P2 -C37 -C36 113.0(13)

C24 -C24A -C25A 103(3) P4 -C39 -C38 113.6(12)

C23A -C24A -C25A 114.2(18) P4 -C41 -C40 116.9(10)

C24 -C24A -C25 87(3) P4 -C43 -C42A 119(2)

C25 -C24A -C25A 16.5(15) P4 -C43 -C42 99(2)

C5 -C6 -H6 119.00 H21 -C21 -H21A 35.00

C7 -C6 -H6 119.00 C22A -C21A -H21 135.00

C9 -C8 -H8 118.00 C22A -C21A -H21A 119.00

C7 -C8 -H8 118.00 N3A -C21A -H21A 119.00

C8 -C9 -H9 119.00 C21 -C21A -H21 31.00

C10 -C9 -H9 119.00 C21 -C21A -H21A 54.00

C11 -C10 -H10 121.00 C22 -C21A -H21 106.00

C9 -C10 -H10 121.00 C22 -C21A -H21A 94.00

C14 -C13 -H13 117.00 N3 -C21A -H21 100.00

C12 -C13 -H13 117.00 N3 -C21A -H21A 119.00

C16 -C15 -H15 118.00 N3A -C21A -H21 100.00

N1 -C15 -H15 118.00 H21 -C21A -H21A 25.00

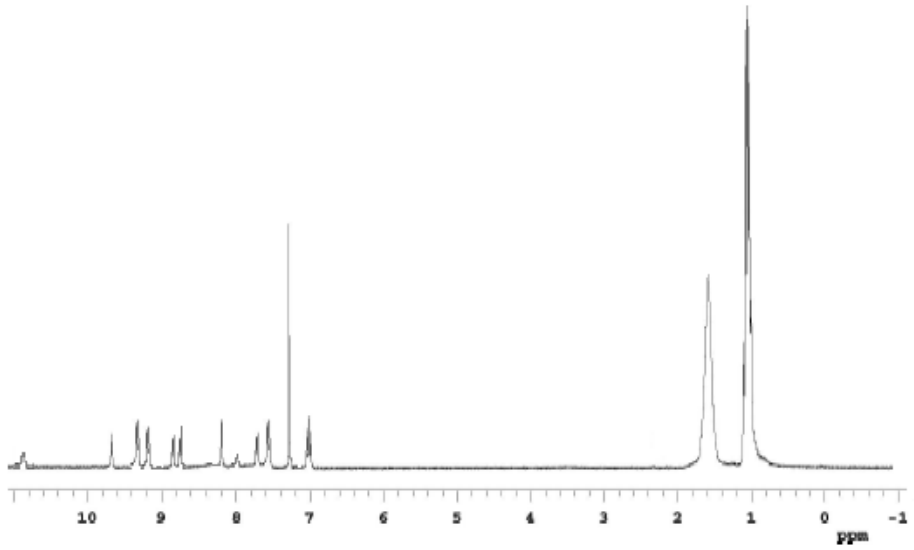
C15 -C16 -H16 121.00 C23 -C22 -H22A 68.00

C17 -C16 -H16 121.00 C21 -C22 -H22 123.00

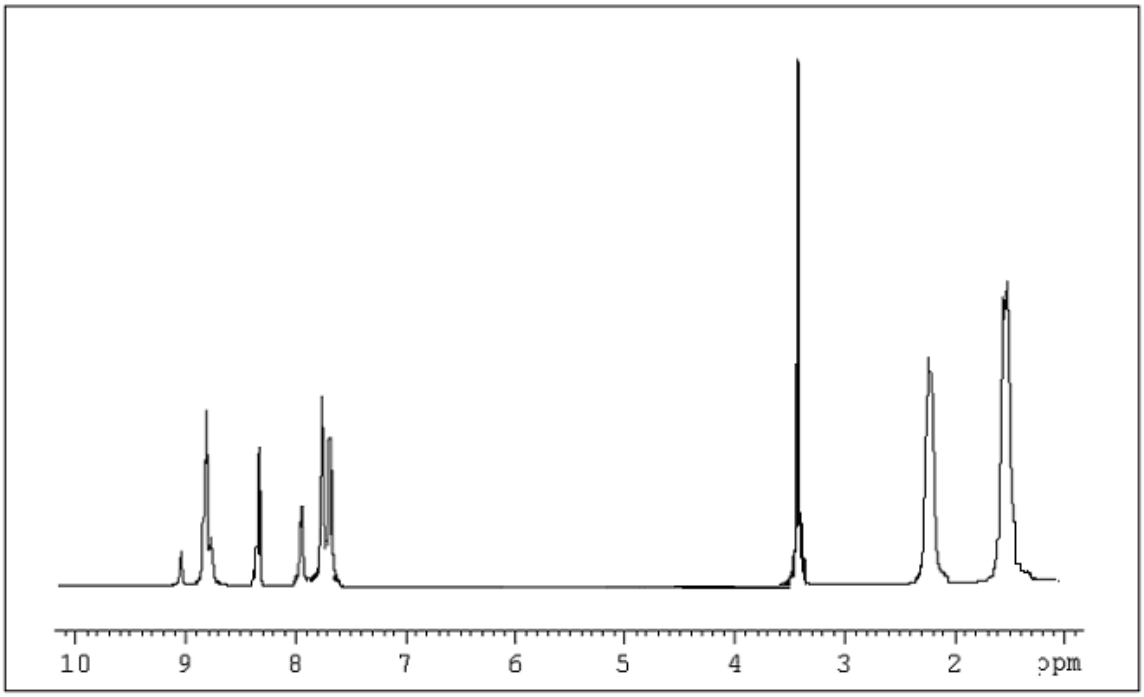
C17 -C18 -H18 122.00 C21 -C22 -H22A 155.00

C19	-C18	-H18	121.00	C21A	-C22	-H22	132.00
C18	-C19	-H19	117.00	C21A	-C22	-H22A	144.00
N1	-C19	-H19	117.00	C22A	-C22	-H22	133.00
N3	-C21	-H21A	131.00	C22A	-C22	-H22A	73.00
N3A	-C21	-H21	116.00	H22	-C22	-H22A	60.00
N3	-C21	-H21	116.00	C23	-C22	-H22	123.00
C21A	-C21	-H21	138.00	C21A	-C22A	-H22A	121.00
C21A	-C21	-H21A	105.00	C22	-C22A	-H22A	62.00
N3A	-C21	-H21A	131.00	C21	-C22A	-H22A	115.00
C22	-C21	-H21	116.00	C23A	-C22A	-H22A	121.00
C22	-C21	-H21A	94.00	C23	-C22A	-H22A	95.00
C22A	-C21	-H21	138.00	N2A	-C23	-H22A	121.00
C22A	-C21	-H21A	108.00	C20	-C23	-H22A	85.00

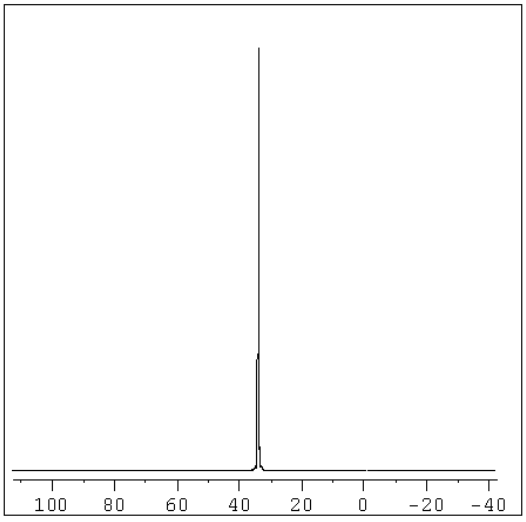
Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z+1



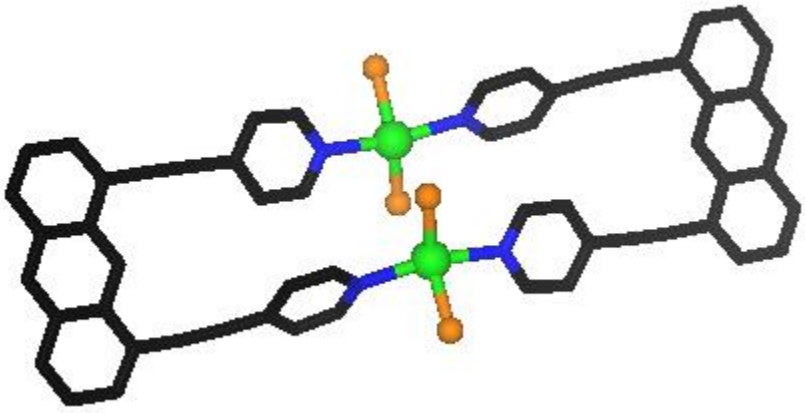
Sup Fig-1: ^{1}H NMR of complex **1**.



Sup-Fig2: ^{1}H NMR of complex-**2**.



Sup-Fig-3: ^{31}P NMR of complex-**2.**



Sup-Fig-4: Proposed molecular view of the rectangle **2**.