Supporting information

Two-dimensional flexible porous coordination polymer based on Co(II) and terpyridyl phosphine oxide

Juan Feng, Hongmiao Li, Qiuli Yang, Shi-Chao Wei, Jianyong Zhang* and Cheng-Yong Su

School of Chemistry and Chemical Engineering, Sun Yat-Sen University, Guangzhou, 510275, China. Tel: 86 20 8411 0539; E-mail: zhjyong@mail.sysu.edu.cn

Characterization data of phosphine oxides.

Py2PO. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.82 (d, J = 3.0 Hz, 4H), 8.11 (d, J = 5.4 Hz, 4H), 8.06 (s, 2H), 7.94–7.84 (m, 4H), 7.79–7.70 (m, 4H), 7.66–7.59 (m, 2H), 7.58–7.50 (m, 4H). ^{31}P{^{1}H} NMR (121 MHz, $CDCl_3$): δ 28.7 (s). TOF-MS (ESI+): m/z found (calcd.) for $[M+H]^+$ ($C_{33}H_{25}N_3PO$) = 510.1777 (510.1730). IR (cm^{-1}, KBr): 3406m, 3053w, 1593s, 1443w, 1386w, 1182m (P=O), 1118s, 1064w, 996w, 822m, 720s, 694m, 694m, 547s.

Py2PO'. ^{1}H NMR (400 MHz, DMSO-d_6): δ 8.83 – 8.77 (d, J = 5.23 Hz, 4H), 8.57 (s, 2H), 8.41–8.34 (d, J = 5.93 Hz, 4H), 8.31–8.25 (d, J = 8.38 Hz, 2H), 8.03–7.94 (m, 4H), 7.80–7.64 (m, 8H), 7.64–7.56 (m, 4H). ^{31}P{^{1}H} NMR (121 MHz, DMSO-d_6): δ 25.4 (s). TOF-MS (ESI+): m/z found (calcd.) for $[M+H]^+$ = 586.2033 (586.2043). IR (cm^{-1}, KBr): 3386m, 3030w, 1593s, 1595s, 1554m, 1490m, 1433m, 1394m, 1314w, 1183s (P=O), 1119s, 1066w, 1000m, 818s, 750m, 725m, 700s, 629m, 557s, 534s.

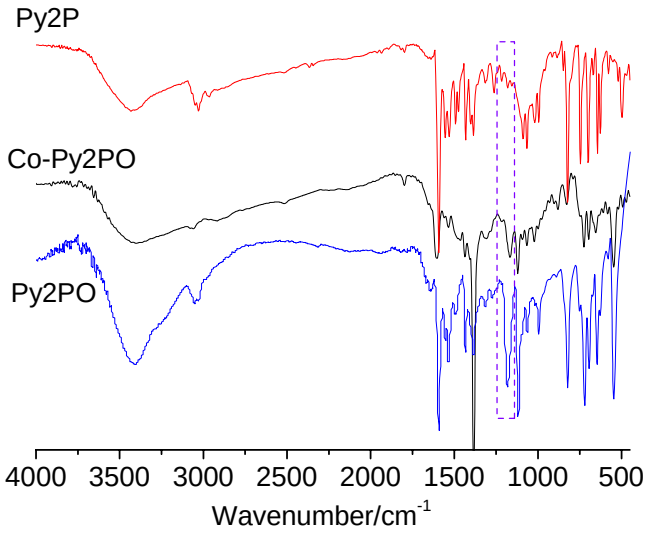

Fig. S1 FT-IR spectra of Py2P, Py2PO and Co-Py2PO (KBr pellets), highlighting the P=O band.

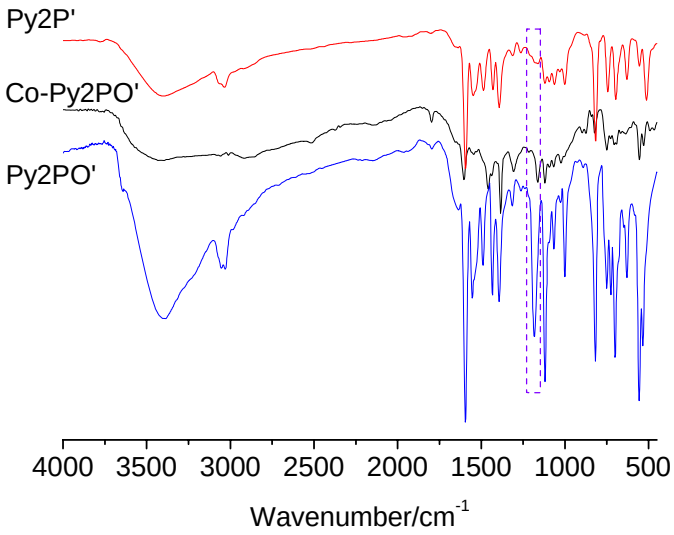

Fig. S2 FT-IR spectra of Py2P', Py2PO' and Co-Py2PO' (KBr pellets), highlighting the P=O band.

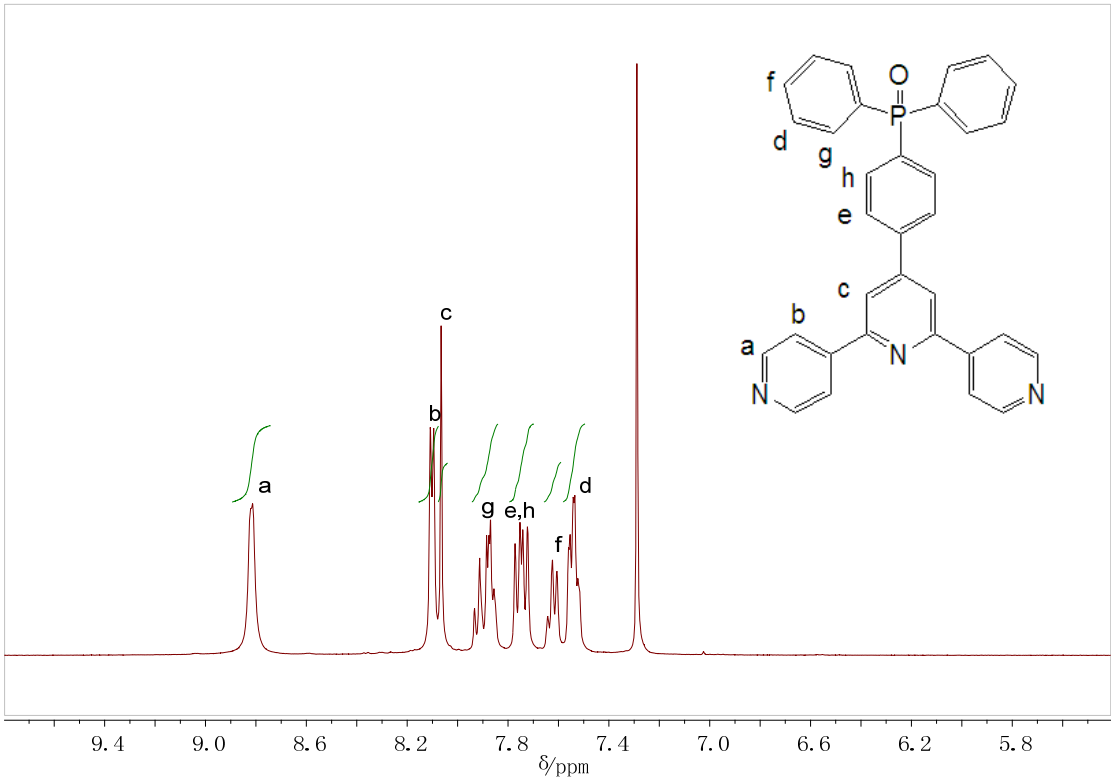

Fig. S3 ^{1}H NMR spectrum of Py2PO in $CDCl_3$.

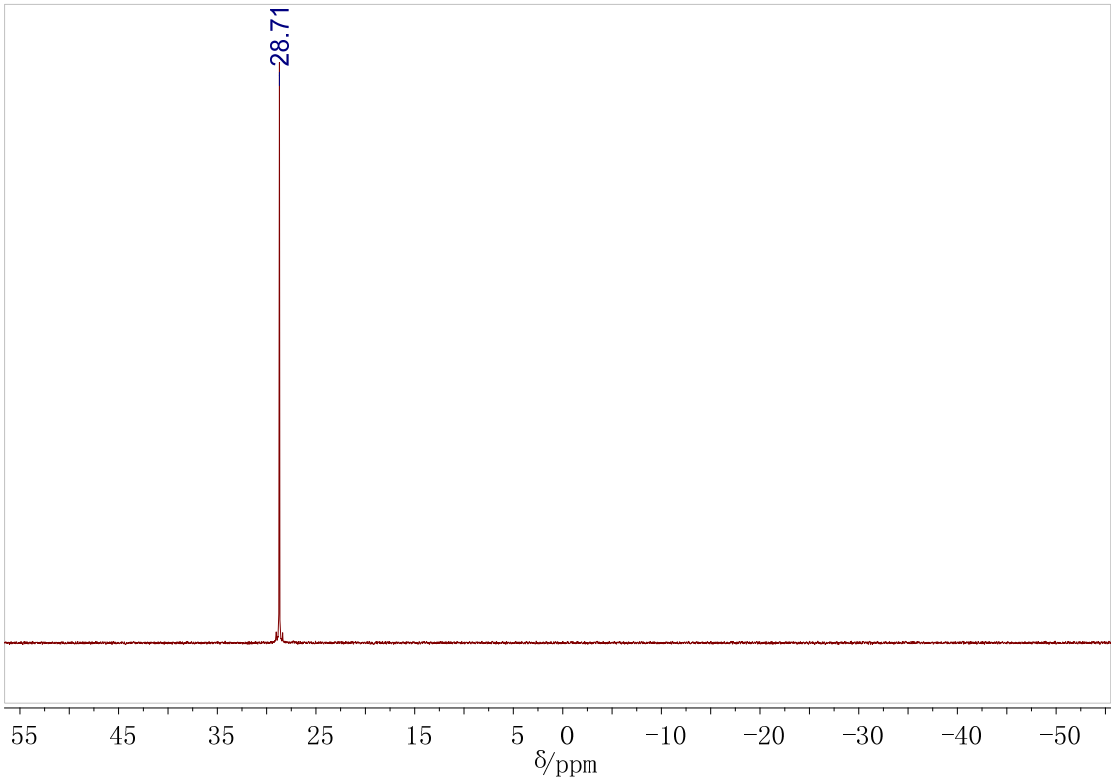

Fig. S4 $^{31}P\{^{1}H\}$ NMR spectrum of Py2PO in $CDCl_3$.

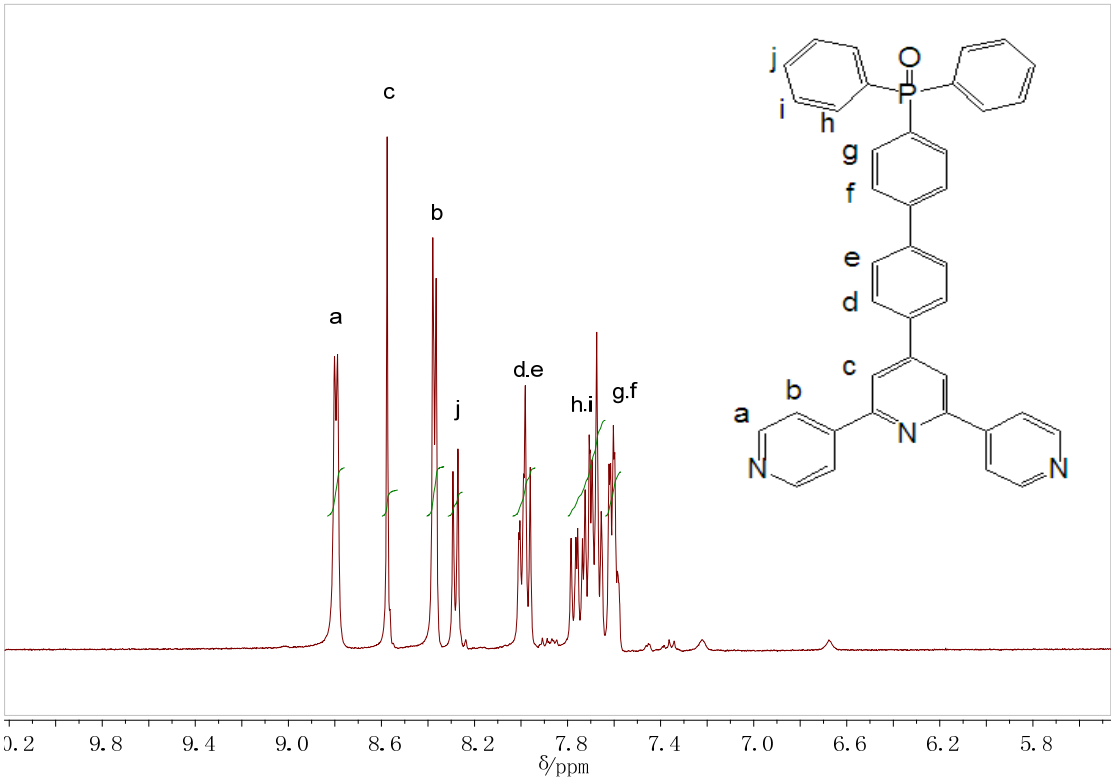

Fig. S5 ^{1}H NMR spectrum of Py2PO' in DMSO-d_6.

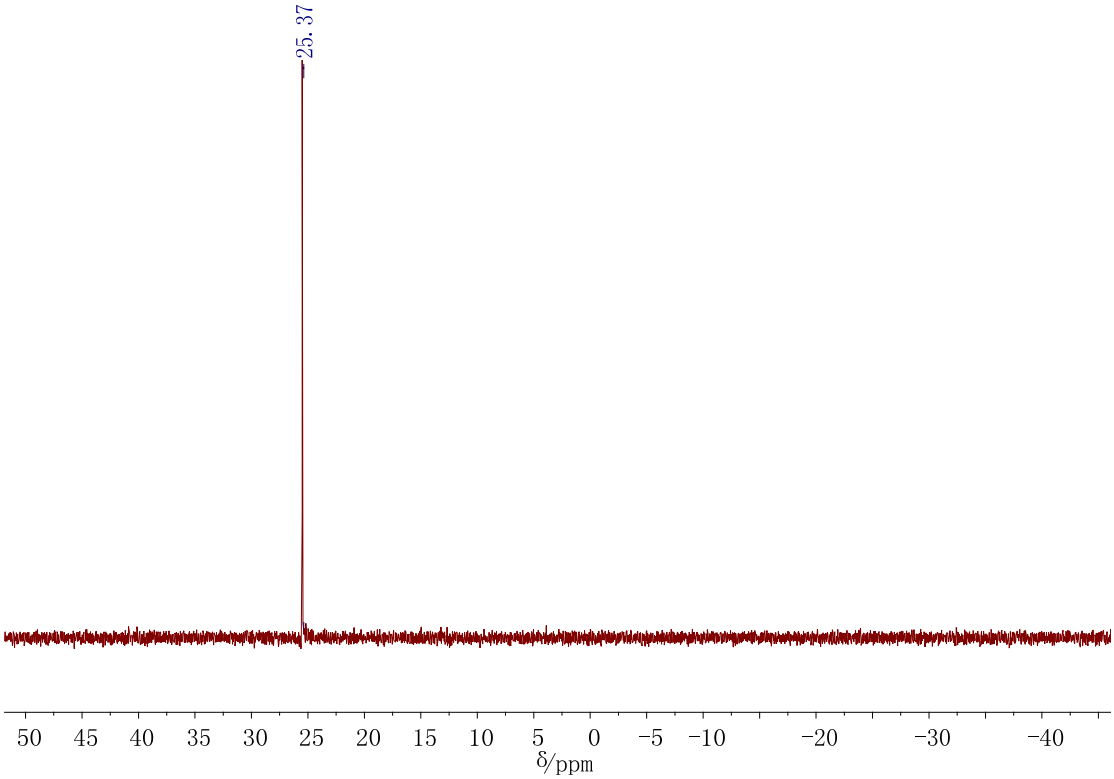

Fig. S6 ^{31}P{^{1}H} NMR spectrum of Py2PO' in DMSO-d_6.

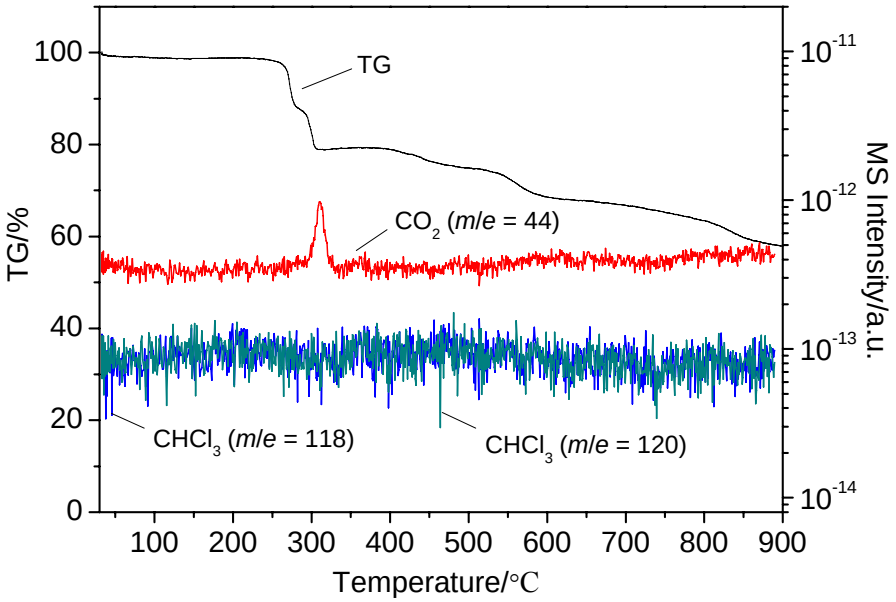

Fig. S7 TG-MS study of Co-Py2PO' showing no loss of solvated $CHCl_3$ molecules.

Table S1 Selected bond lengths (Å) and angles (°) for Co-Py2PO.

Bond length/Å			
Co(1)-O(6)	2.057(3)	Co(2)-N(1)	2.119(4)
Co(1)-O(1)	2.062(4)	Co(2)-N(6)#3	2.120(4)
Co(1)-N(4)	2.099(4)	Co(2)-O(12)	2.149(4)
Co(1)-N(3)#1	2.144(4)	Co(2)-O(13)	2.242(4)
Co(1)-O(3)	2.171(3)	N(3)-Co(1)#4	2.144(4)
Co(1)-O(5)	2.223(3)	N(6)-Co(2)#5	2.120(4)
Co(2)-O(2)#2	2.023(3)	O(2)-Co(2)#6	2.023(3)
Co(2)-O(9)	2.107(4)		
Bond angle/°			
O(6)-Co(1)-O(1)	92.91(14)	O(2)#2-Co(2)-N(1)	176.26(14)
O(6)-Co(1)-N(4)	95.50(15)	O(9)-Co(2)-N(1)	86.28(14)
O(1)-Co(1)-N(4)	171.58(14)	O(2)#2-Co(2)-N(6)#3	86.42(13)
O(6)-Co(1)-N(3)#1	89.59(13)	O(9)-Co(2)-N(6)#3	88.48(15)
O(1)-Co(1)-N(3)#1	84.78(15)	N(1)-Co(2)-N(6)#3	97.31(14)
N(4)-Co(1)-N(3)#1	95.72(15)	O(2)#2-Co(2)-O(12)	92.36(13)
O(6)-Co(1)-O(3)	173.10(13)	O(9)-Co(2)-O(12)	174.05(13)
O(1)-Co(1)-O(3)	86.52(14)	N(1)-Co(2)-O(12)	87.93(14)
N(4)-Co(1)-O(3)	85.08(15)	N(6)#3-Co(2)-O(12)	90.92(15)
N(3)#1-Co(1)-O(3)	97.20(14)	O(2)#2-Co(2)-O(13)	90.81(13)
O(6)-Co(1)-O(5)	113.93(13)	O(9)-Co(2)-O(13)	122.68(14)
O(1)-Co(1)-O(5)	85.39(14)	N(1)-Co(2)-O(13)	86.17(14)
N(4)-Co(1)-O(5)	90.77(14)	N(6)#3-Co(2)-O(13)	148.84(15)
N(3)#1-Co(1)-O(5)	154.91(14)	O(12)-Co(2)-O(13)	58.15(14)
O(3)-Co(1)-O(5)	59.17(13)	O(2)#2-Co(2)-O(9)	93.51(14)

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

Table S2 Selected bond lengths (Å) and angles (°) for Co-Py2PO'.

Bond length/Å			
Co(1)-O(1)#1	2.083(6)	Co(1)-N(1)	2.114(5)
Co(1)-O(5)	2.162(6)	Co(1)-N(3)#3	2.120(5)
Co(1)-O(2)	2.196(6)	N(3)-Co(1)#4	2.120(5)
Co(1)-O(3)	2.302(9)	O(1)-Co(1)#2	2.083(6)
Bond angle/°			
O(1)#1-Co(1)-N(1)	92.3(2)	N(3)#3-Co(1)-O(2)	90.3(2)
O(1)#1-Co(1)-N(3)#3	91.6(2)	O(5)-Co(1)-O(2)	177.9(3)
N(1)-Co(1)-N(3)#3	175.6(2)	O(1)#1-Co(1)-O(3)	141.3(3)
O(1)#1-Co(1)-O(5)	95.9(2)	N(1)-Co(1)-O(3)	85.3(3)
N(1)-Co(1)-O(5)	86.0(2)	N(3)#3-Co(1)-O(3)	92.8(3)
N(3)#3-Co(1)-O(5)	91.6(2)	O(5)-Co(1)-O(3)	122.4(3)
O(1)#1-Co(1)-O(2)	84.9(2)	O(2)-Co(1)-O(3)	56.7(2)
N(1)-Co(1)-O(2)	92.0(2)		

Symmetry transformations: #1: 1-*x*, 1-*y*, *z*+1/2 #2: 1-*x*, 1-*y*, *z*-1/2 #3: *x*-1/2, -*y*-1/2, *z* #4: *x*+1/2, -*y*-1/2, *z*.