Electronic Supplementary Material (ESI) for CrystEngComm.

Contents

1 Experimental....2
1.1 Materials and physical measurements....2
1.2 Synthesis of compound 1....2
1.3 X-Ray crystallography....3
Fig.S1 The double helix chains of carboxyl which around Ag ions (left: $P6_122$, right: $P6_522$). 4
Fig.S2 The nitro of 5-nip display a helix running along the 6_1 or 6_5 screw axis (left: $P6_122$, right: $P6_522$). 5
Fig.S3 View of the topological net in ab plane. 6
Fig.S4 The powder X-ray diffraction patterns of 1P ($P6_122$) and 1M ($P6_522$). 7
Fig.S5 The IR spectra of compound 1. 8
Fig.S6 The photoluminescence spectra of compound 1 and free ligands. 9
Fig.S7 The TG curve for complex 1. 10
Table S1 Crystallographic data for complex 1....11
Table S2 Selected bond distances (Å) and angles (°) for **1**....12

1 Experimental

1.1 Materials and physical measurements

All starting materials and solvents which used in these synthetic reactions are purchased commercially and were used as obtained from the supplier without further purification. IR spectra were carried out on a Nicolet Avatar 330 FITR Spectrometer as KBr pellets in the frequency range of Elemental analyses for 4000–400 cm^{-1}. Vibrational circular dichroism spectra were recorded on a Chiral IR-2X instrument using KBr. Thermogravimetic analyses were performed on a SDT Q600 instrument from 30 to 800 ˚C at a heating rate of 10 ˚C min^{-1} under N_2 atmosphere (100ml min^{-1}). Elemental analyses for C, H, N were measured on a CE instruments Ea 1110 elemental analyzer. X-ray powder diffractions were measured on a Panalytical X-Pert pro diffractometer with Cu- Kα radiation. Photoluminescent properties were performed on a Hitachi F-7000 Fluorescence Spectrophotometer with solid powder on a 1cm quarts round plate.

1.2 Synthesis of compound 1

A mixture of aqueous solution $AgNO_3$ (34.2 mg $AgNO_3$ (0.2 mmol) dissolve in 100μml water), mpyz (272.2 mg, 0.2 mmol) and H_2npt (422.3 mg, 0.2 mmol) took place in CH_3CN – DMF (N,N-Dimethylformamide)

mixed solvent (6 mL, *v*/*v*: 3/3) in the presence of ammonia (14M, 20d) under ultrasonic treatment (160W, 40KHz,30min) at 40 °C. The resultant solution was allowed to evaporate slowly in darkness at room temperature for several days to give plate-colorless crystals of **1** (Yield: 54%, based on Ag). Anal. Calc. (found) for $Ag_2C_{16}H_{15}N_3O_6$: C, 34.22 (34.54); H, 2.67 (2.65); O, 17.11 (17.28); N,7.49 7.45)%. IR (KBr): ν(cm^{-1}) = 3419 (m), 3085 (w), 2917 (w), 2848 (w), 1697 (m), 1619 (s), 1598 (m), 1571 (w), 1506 (s), 1444 (w), 1425 (w), 1362 (s), 1193 (w), 1081 (w), 924 (w), 793 (m), 740 (m), 715 (m), 530 (w).

1.3 X-Ray crystallography

Crystallographic data of compounds **1P and 1M** were collected on Rigaku R-AXIS RAPID imaging Plate single-crystal diffractometer with graphite-monochromated Mo-Kα radiation source (λ=0.71073 Å) operating at 50 kV and 90 mA in ω scan mode. The crystal structures were solved and refined using Fullmatrix least-squares based on F2 with program SHELXS-97 and SHELXL-97 within OLEX2. Absorption correction was applied by correction of symmetry-equivalent reflections using the ABSCOR program. In all cases, the highest possible space group was chosen. Hydrogen atoms were placed in calculated positions and included as riding atoms with isotropic displacement parameters 1.2–1.5 times Ueq of the attached C or N atoms.

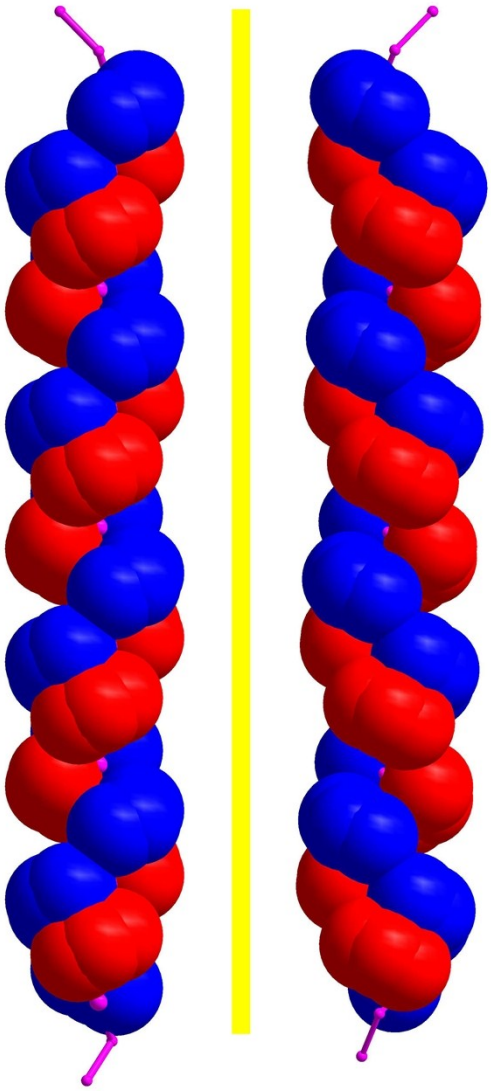

Fig.S1 The double helix chains of carboxyl which around Ag ions (left: $P6_122$, right: $P6_522$).

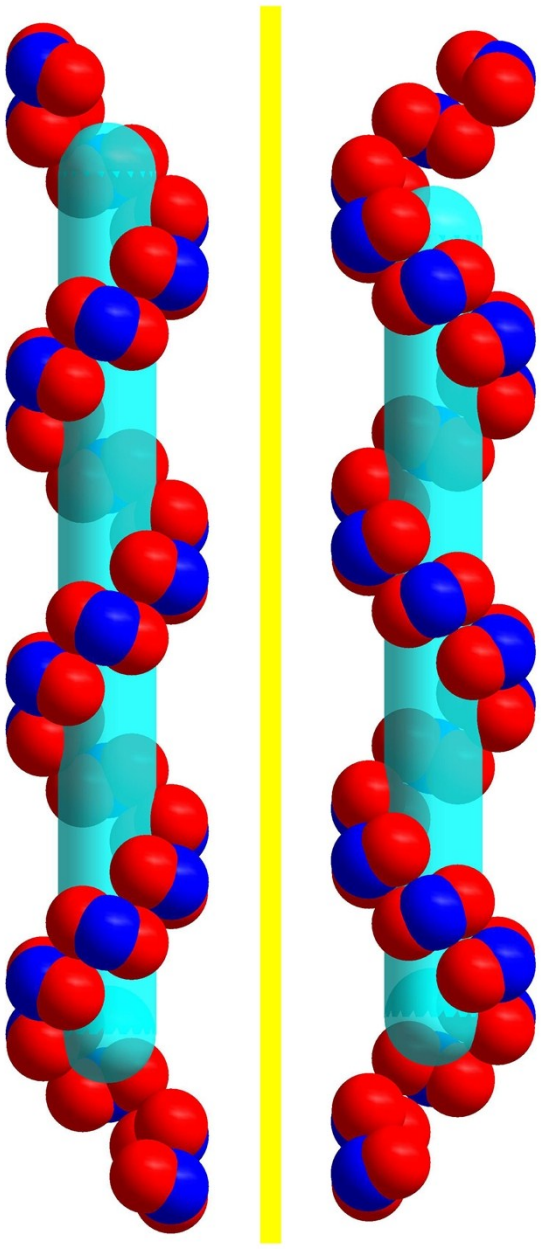

Fig.S2 The nitro of 5-nip display a helix running along the 6_1 or 6_5 screw axis (left: $P6_122$, right: $P6_522$).

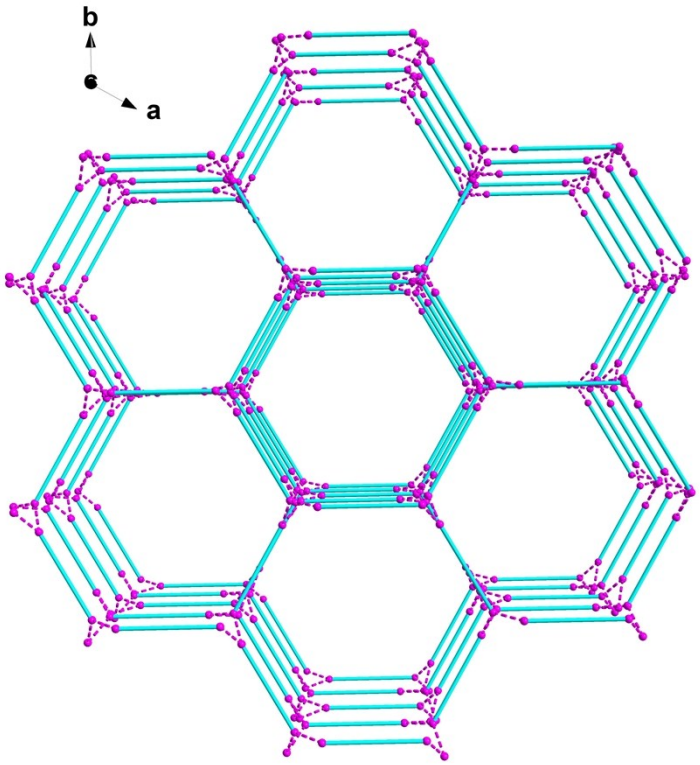

Fig.S3 View of the topological net in ab plane.

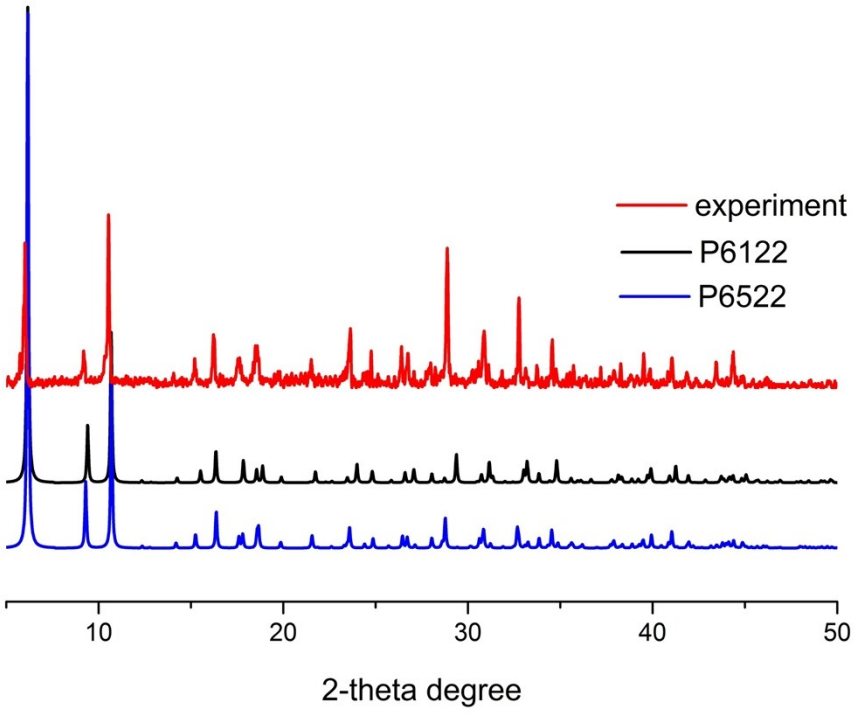

Fig.S4 The powder X-ray diffraction patterns of **1P** ($P6_122$) and **1M** ($P6_522$).

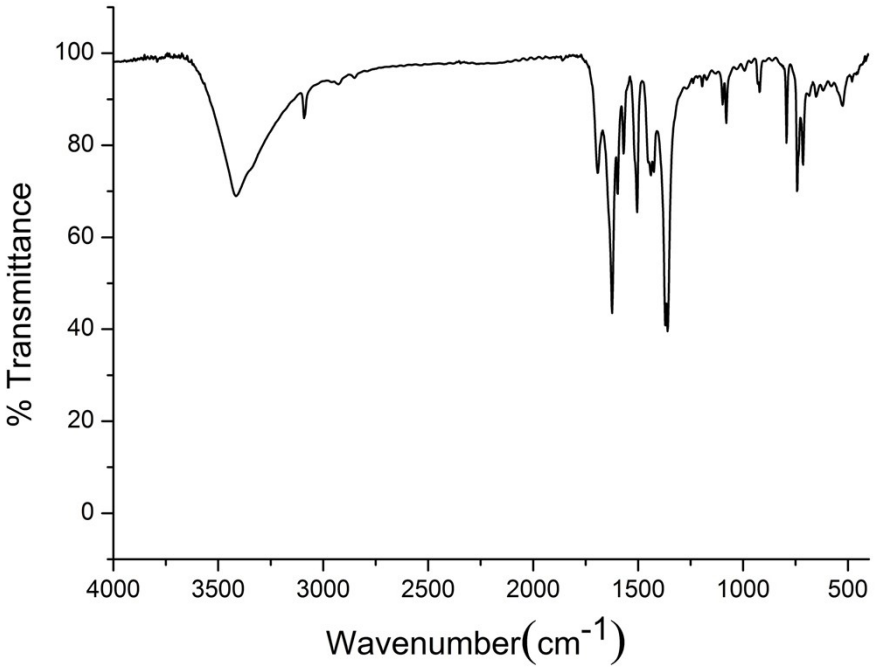

Fig.S5 The IR spectra of compound **1**.

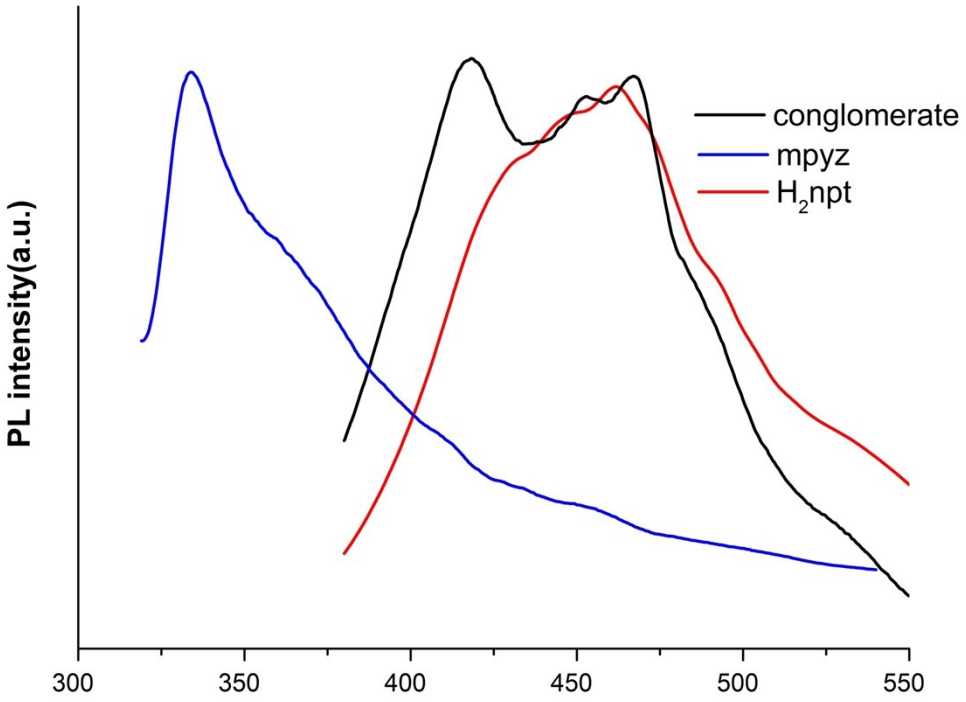

Fig.S6 The photoluminescence spectra of compound **1** and free ligands.

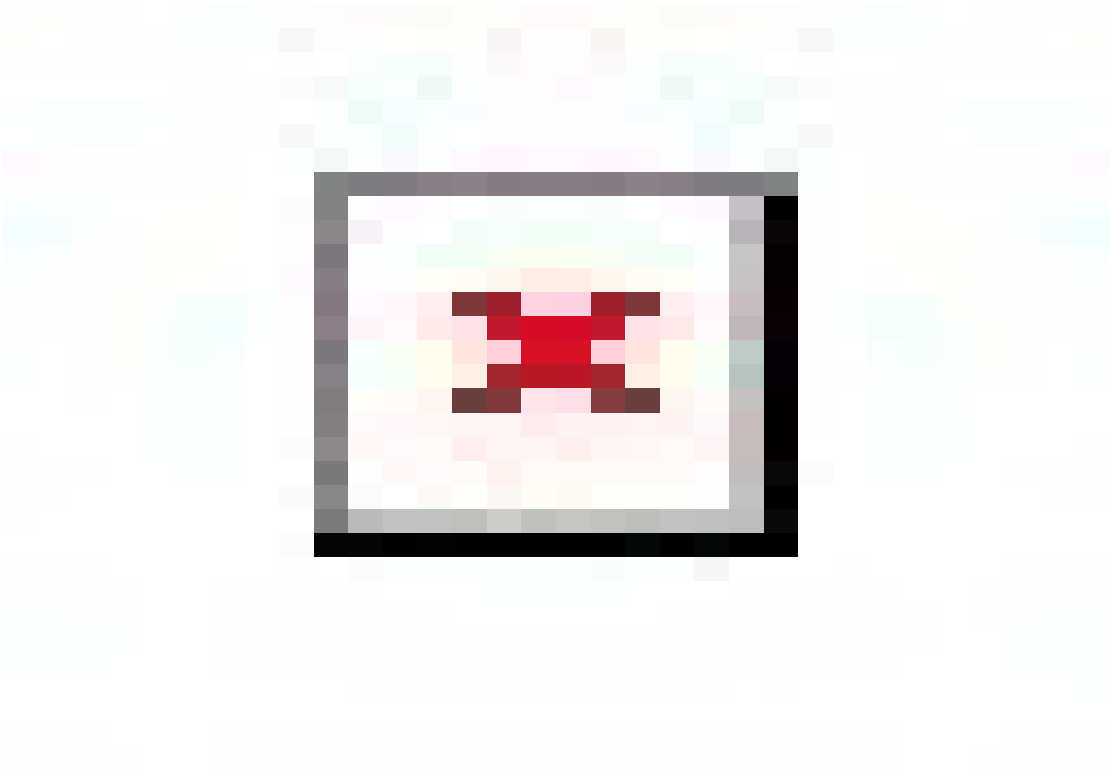

Fig.S7 The TG curve for complex **1**.

As shown in Fig.S8 , complexes underwent a 22.06% mass decrease from ~100 to ~250 ˚C, corresponding to the mpyz ligand which calculated value is 24.04%. And the residue composition of this compound is then decomposed in thr temperature arranged of ~250 to~ 800 ˚C.

Table S1 Crystallographic data for complex 1

Complexes	**1P**	**1M**
Formula	$Ag_2C_{16}H_{15}N_3O_6$	$Ag_2C_{16}H_{15}N_3O_6$
M_r	561.05	561.05
Crystal system	hexagonal	hexagonal
Space group	$P6_122$	$P6_522$
a (Å)	16.5479(10)	16.5272(5)
b (Å)	16.5479(12)	16. 5272(5)
c (Å)	12.4353(15)	12. 7024(3)
α (deg)	90.00	90.00
β (deg)	90.00	90.00
γ (deg)	120.00	120.00
Z	6	6
V (Å^3)	2949.0(4)	3004.79(17)
D_c(g cm^{-3})	1.8954	1.8602
μ(mm^{-1})	2.028	16.015
F(000)	1634	1651
no. of unique reflns	28961	5850
no. of obsd reflns[$I > 2\sigma(I)$]	2260	1682
Parameters	127	127
GOF	1.031	1.030
Final R indices [$I > 2\sigma(I)$][a,b]	$R_1 = 0.0557$, $wR_2 = 0.1432$	$R_1 = 0.0467$ $wR_2 = 0.1431$
R indices (all data)	$R_1 = 0.0615$, $wR_2 = 0.1469$	$R_1 = 0.0557$ $wR_2 = 0.1545$
Largest difference peak and hole (e Å^{-3})	0.80 and -1.26	1.27 and -0.98
Flack parameter	0.04(11)	-0.00(3)

[a]$R_1 = \sum||F_o| - |F_c||/\sum|F_o|$. [b]$wR_2 = [\sum w(F_o^2 - F_c^2)^2/\sum w(F_o^2)^2]^{0.5}$.

Table S2 Selected bond distances (Å) and angles (°) for **1**

Complex **1P**			
Ag1—N1	2.242 (8)	O1^{v}—Ag1—N1	125.75 (15)
Ag1—O1^{iv}	2.411 (5)	O1^{iv}—Ag1—N1	125.75 (15)
Ag1—O1^{v}	2.411 (5)	O1^{v}—Ag1—O1^{iv}	108.5 (3)
Ag2—N2	2.344 (8)	O2^{iii}—Ag2—N2	114.11 (16)
Ag2—O2	2.261 (5)	O2—Ag2—N2	114.11 (16)
Ag2—O2^{iii}	2.261 (5)	O2^{iii}—Ag2—O2	131.8 (3)
Complex **1M**			
Ag1—N1	2.269 (9)	O1^{v}—Ag1—N1	125.55 (18)
Ag1—O1^{iv}	2.422 (6)	O1^{iv}—Ag1—N1	125.55 (18)
Ag1—O1^{v}	2.422 (6)	O1^{v}—Ag1—O1^{iv}	108.9 (4)
Ag2—N2	2.319 (8)	O2—Ag2—N2	114.6 (2)
Ag2—O2^{iii}	2.255 (6)	O2^{iii}—Ag2—N2	114.6 (2)
Ag2—O2	2.255 (6)	O2^{iii}—Ag2—O2	130.9 (4)

Complex **1P**: (i) *y*, −*x*+*y*+1, *z*−1/6; (ii) *x*−*y*, *x*, *z*+1/6; (iii) −*y*+1, −*x*+1, −*z*+5/6; (iv) −*x*+1, −*x*+*y*, −*z*+2/3; (v) *x*−*y*+1, *x*, *z*+1/6; (vi) −*x*, −*x*+*y*, −*z*+2/3; (vii) *y*, −*x*+*y*, *z*−1/6; (viii) −*x*+1, −*x*+*y*+1, −*z*+2/3.

Complex **1M**: (i) *y*, −*x*+*y*+1, *z*+1/6; (ii) *x*−*y*, *x*, *z*−1/6; (iii) −*y*+1, −*x*+1, −*z*+7/6; (iv) *x*−*y*+1, −*y*+1, −*z*+1; (v) *y*, −*x*+*y*, *z*+1/6; (vi) *x*−*y*+1, −*y*+2, −*z*+1; (vii) *x*−*y*+1, *x*, *z*−1/6; (viii) *x*−*y*, −*y*+1, −*z*+1.