Two New Silver Coordination Polymers Constructed from 3,3-Azodibenzoic Acid and Different Pyridine Derivatives: Syntheses, Structures and Fluorescent Properties Postprint

Authors: HOU Xiang-Yang, WANG Xiao, REN Yi-Xia, TANG Long, JU Ping, WANG Ji-Jiang, KANG Wei-Wei, LIU Xiao-Li

Date: 2017-11-05T00:00:00+00:00

Abstract

Two coordination polymers (CPs), {[Ag(ADA)0.5(DPE)]·H2O}n (1) and {[Ag(ADA)0.5(Bipy)0.5]·H2O}n (2), (H2ADA = 3,3-azodibenzoic acid, DPE = 1,2-di(4-pyridyl)- ethylene, Bipy = 4,4 -bipyridine), have been synthesized via solvothermal reactions of Ag+ with ADA2- and/or DPE, Bipy. CPs 1 and 2 were characterized by elemental analyses, IR spectra, thermal behaviors, and X-ray single-crystal diffraction. CPs 1 and 2 feature "Ag··· Ag" subunits. CP 1 shows a 3D construction, in which the "Ag··· Ag" subunits extend through ADA2- and DPE ligands using 6-kO,O;kO;kO;kO,O;kO;kO and 2-kO;kO coordination modes, respectively. It crystallizes in triclinic system, space group P, with a = 0.3808(18), b = 1.2476(6), c = 1.309(6) nm, = 76.757(5), = 84.649(5), = 86.809(5)º, V = 0.6024(5) nm3, Z = 2, Mr = 351.11, C13H11AgN2O3, Dc = 1.936 g/cm3, F(000) = 348, S = 1.064, R = 0.0323 and wR = 0.0689. CP 2 exhibits a 3D supramolecular structure, in which the "Ag··· Ag" subunits are connected by ADA2- and DPE ligands with 6-kO;kO;kO,O;kO;kO and 2-kO;kO coordination modes, respectively. Ultimately, through hydrogen bond and ··· interaction, the "Ag··· Ag" subunits stabilize the 3D supramolecular structure of 2. It crystallizes in monoclinic, space group C2/c, with a = 25.301(15), b = 13.197(8), c = 6.970(4) nm, = 102.597(7)º, V = 2.271(2) nm3, Z = 8, C12H10AgN2O2.50, Mr = 330.09, Dc = 1.931 g/cm3, F(000) = 1304, S = 1.082, R = 0.1107 and wR = 0.2984. The fluorescence properties of CPs 1 and 2 have been also investigated.

Full Text

Preamble

Two New Silver Coordination Polymers Constructed from 3,3-Azodibenzoic Acid and Different Pyridine Derivatives: Syntheses, Structures and Fluorescent Properties

Xiang-Yang Hou, Xiao Wang, Yi-Xia Ren, Long Tang, Ping Ju, Ji-Jiang Wang, Wei-Wei Kang, Xiao-Li Liu

Department of Chemistry and Chemical Engineering, Yan' an University Laboratory of New Energy & New Function Materials, Yan' an Key Laboratory of Analytical Technology and Detection, Yan' an University, Shaanxi 716000, China

Abstract

Two coordination polymers (CPs), {[Ag(ADA)0.5(DPE)]·H2O}n (1) and {[Ag(ADA)0.5(Bipy)0.5]·H2O}n (2), where H2ADA = 3,3-azodibenzoic acid, DPE = 1,2-di(4-pyridyl)ethylene, and Bipy = 4,4' -bipyridine, have been synthesized via solvothermal reactions of Ag+ with ADA2- and DPE or Bipy. CPs 1 and 2 were characterized by elemental analysis, IR spectroscopy, thermal analysis, and single-crystal X-ray diffraction. Both CPs feature Ag···Ag subunits.

CP 1 exhibits a three-dimensional framework structure in which the Ag···Ag subunits are extended through ADA2- and DPE ligands adopting 6-kO,O;kO;kO;kO,O;kO;kO and 2-kO;kO coordination modes, respectively. It crystallizes in the triclinic space group P , with unit cell parameters a = 0.3808(18), b = 1.2476(6), c = 1.309(6) nm, = 76.757(5)°, = 84.649(5)°, = 86.809(5)°, V = 0.6024(5) nm^3, Z = 2, Mr = 351.11, formula C13H11AgN2O3, Dc = 1.936 g/cm^3, F(000) = 348, S = 1.064, R = 0.0323 and wR = 0.0689.

CP 2 displays a three-dimensional supramolecular structure in which the Ag···Ag subunits are connected by ADA2- and Bipy ligands with 6-kO,O;kO;kO;kO,O;kO;kO and 2-kO;kO coordination modes, respectively. Ultimately, hydrogen bonding and ··· interactions stabilize the three-dimensional supramolecular structure of 2. It crystallizes in the monoclinic space group C2/c, with a = 25.301(15), b = 13.197(8), c = 6.970(4) nm, = 102.597(7)°, V = 2.271(2) nm^3, Z = 8, formula C12H10AgN2O2.50, Mr = 330.09, Dc = 1.931 g/cm^3, F(000) = 1304, S = 1.082, R = 0.1107 and wR = 0.2984. The fluorescence properties of CPs 1 and 2 have also been investigated.

Keywords: silver; coordination polymers; synthesis; structure; fluorescence properties

1. Introduction

In recent years, the construction of coordination polymers (CPs) has primarily depended on the balance between metal ions and multidentate ligands under suitable reaction conditions, including temperature, pressure, and solvent [1-3]. However, the structures of CPs based on flexible ligands are difficult to predict due to their conformational diversity under different reaction conditions, and the resulting architectures are largely considered serendipitous [4,5]. In fact, the architectures of CPs can be achieved through ligands containing flexible structural units such as "-X-X-" (where X = C, N, O, etc.). To date, many types of flexible ligands with "-X-X-" units have been reported in combination with metal ions, including documented CPs with flexible "-C-C-" type ligands [6].

A series of CPs have been synthesized using 3,3' - and 4,4' -dithiobisbenzoic acid ligands containing "-S-S-" units [7], while biphenylethene-4,4'-dicarboxylate ligands with "-C=C-" units have been used to bridge Zn^{2} or Cd^{2} centers in previous studies [8]. Recently, a sequence of compounds with flexible ligands containing "-N=N-" units has also been reported [9]. In particular, imidazole and pyridine-based flexible ligands containing "-X-X-" or "-X-X-X-" units that bridge metal ion centers in complex synthesis have been documented [10-15]. Such flexible units in ligands can give rise to frameworks with diverse structures.

Metallic silver and its complexes, as novel functional materials, have potential applications in medicine, fluorescence, ion exchange, catalysis, gas adsorption and separation, among other areas [16-19]. Recently, research on the fluorescent properties of silver complexes has become relatively extensive. To achieve useful luminescent Ag-CPs, an effective method is to employ a ligand-based strategy utilizing -conjugated rigid organic ligands. To date, various luminescent Ag-CPs have been reported based on organic molecules; however, most have focused on rigid ligands, with only a few Ag-CPs investigated based on ligands containing flexible "-X-X-" structural units.

Building upon these ideas and leveraging the structural and property advantages of Ag-CPs, this work selected 3,3-azodibenzoic acid and/or 1,2-di(4-pyridyl)ethylene and 4,4' -bipyridine as ligands. Through solvothermal reactions of these mixed ligands with AgNO under different mixed solvent systems, pressures, and temperatures, we successfully synthesized two new CPs: {[Ag(ADA)0.5(DPE)] · H O}n (1) and {[Ag(ADA)0.5(Bipy)0.5] · H O}n (2). These compounds were characterized by elemental analysis, single-crystal X-ray diffraction, IR spectroscopy, and thermogravimetric analysis. Additionally, the fluorescence properties of 1 and 2 were investigated in the solid state at room temperature.

2. Experimental

2.1 Materials and Methods

All solvents and starting materials of analytical grade used in the experiments were purchased commercially and used without further purification. Elemental analysis (C, H, N) was performed on a Perkin-Elmer 2400 elemental analyzer. Infrared spectra were recorded in the range of 4000–400 cm ^{1} on a Bruker EQUINOX-55 spectrophotometer using KBr pellets. Thermal decomposition behavior was investigated under nitrogen atmosphere at a heating rate of 10 °C · min ^{1} using a NETZSCH STA 449C thermogravimetric analyzer. Photoluminescence measurements of the solid samples were conducted on an Edinburgh Instruments FLS920 fluorescence spectrometer at ambient temperature.

2.2 Syntheses

{[Ag(ADA)0.5(DPE)] · H2O}n (1)

A mixture of H ADA (0.1 mmol), DPE (0.13 mmol), AgNO (0.2 mmol), and 15 mL deionized water was sealed in a 25 mL Teflon-lined stainless-steel autoclave. After stirring for 30 minutes at room temperature, the mixture was heated at 160 °C for 96 hours under autogenous pressure and then cooled to room temperature at a rate of 2 °C · h ^{1}. Colorless bulk crystals were collected in 43% yield (based on Ag). Elemental analysis calculated (%) for C H AgN O (1): H, 3.16; C, 44.47; N, 7.98. Found (%): H, 3.12; C, 44.52; N, [value missing in original].

{[Ag(ADA)0.5(Bipy)0.5] · H2O}n (2)

A mixture of H ADA (0.1 mmol), Bipy (0.13 mmol), AgNO (0.2 mmol), and 15 mL water was sealed in a 25 mL Teflon-lined stainless-steel vessel and heated at 170 °C for 3 days under autogenous pressure, then cooled to room temperature at a rate of 5 °C · h ^{1}. Colorless bulk crystals of 2 were obtained in 30% yield (based on Ag). Elemental analysis calculated (%) for C H AgN O . 5: C, 43.66; H, 3.05; N, 8.49. Found (%): C, 43.70; H, 3.10; N, 8.43.

2.3 X-ray Crystal Structure Determination

Crystallographic data for CPs 1 and 2 were collected on a Bruker Smart CCD X-ray diffractometer equipped with graphite-monochromatized MoKa radiation using -scan mode. A semi-empirical absorption correction was applied using the SADABS program [20]. The structures were solved by direct methods and refined on F^{2} by full-matrix least-squares using SHELX-97 [21,22]. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms of coordinated and uncoordinated water molecules were located in difference Fourier maps, while other hydrogen atoms were included in calculated positions and refined with isotropic thermal parameters riding on their parent atoms. Selected bond lengths and bond angles for CPs 1 and 2 are listed in Table 1 .

3. Results and Discussion

3.1 Crystal Structure of CP {[Ag(ADA)0.5(DPE)] · H2O}n (1)

CP 1 crystallizes in the triclinic space group P. As shown in Fig. 1a [Figure 1: see original paper], the asymmetric unit of CP 1 contains one Ag ion, one-half of an ADA^2 anionic ligand, one DPE ligand, and one coordinated water molecule. Each Ag ion is five-coordinated in a distorted tetragonal pyramidal geometry by four oxygen atoms (O(1), O(1)#1, O(1)#2, O(2)) from three ADA^2 anionic ligands and one nitrogen atom (N(2)) from a DPE ligand. One oxygen atom (O(1)#1) occupies the vertex position of the tetragonal pyramid. The Ag-O/N bond lengths are 2.420(3), 2.375(3), 2.600(3), 2.738(3), and 2.243(3) Å, respectively, all of which are consistent with those reported for similar CPs [23]. Notably, each Ag ion is connected by three oxygen atoms (O(1), O(1)#1, O(1)#2) to form a one-dimensional ladder-like chain with Ag···Ag separations of 3.1365(10) and 3.7484(11) Å, indicating weak Ag···Ag interactions in the 1D chain [23]. Furthermore, each ADA^2 anionic ligand adopts a 6-kO,O:kO:kO:kO,O:kO:kO coordination mode, linking adjacent 1D chains through Ag centers to generate a two-dimensional structure in the ac-plane (Fig. 1b [Figure 1: see original paper]). The DPE ligands adopt a 2-kO:kO coordination mode to connect adjacent 2D structures. Thus, the Ag centers, 6-connected ADA^2 ligands, and 2-connected DPE ligands collectively form a three-dimensional framework for CP 1 (Fig. 1c [Figure 1: see original paper]).

3.2 Crystal Structure of {[Ag(ADA)0.5(Bipy)0.5] · H2O}n (2)

X-ray single-crystal diffraction analysis reveals that CP 2 possesses a two-dimensional structure that extends into a three-dimensional supramolecular compound through hydrogen bonding and · · · interactions. CP 2 crystallizes in the monoclinic space group C2/c. The asymmetric unit of CP 2 consists of one Ag ion, one-half of an ADA^2 ligand, one Bipy ligand, and one uncoordinated water molecule (Fig. 2a [Figure 2: see original paper]). Each Ag ion is five-coordinated by one N(2) atom from a Bipy ligand, three carboxylate oxygen atoms (O(1), O(1)#2, O(2)#1) from three ADA^2 ligands, and one Ag(1)#1 ion. The coordination geometry of each Ag ion can be described as a slightly distorted tetragonal pyramid, with four atoms (O(1)#1, O(2)#1, Ag(1)#1, N(2)) occupying the basal positions. The Ag-O/N bond lengths range from 2.234(8) to 2.913(2) Å, and the Ag-Ag bond length is 2.892(2) Å, all of which are consistent with values reported for similar CPs [23]. As shown in Fig. 2b [Figure 2: see original paper], the Ag-Ag units are bridged by carboxylate oxygen atoms (O(1)-C(1)-O(2)) of ADA^2 ligands to form one-dimensional chains containing eight-membered rings along the c-axis direction, with the shortest distance for the eight-membered rings being 14.6184(61) Å in the same plane. Adjacent 1D chains are linked by ADA^2 and Bipy ligands adopting 6-kO,O:kO:kO:kO,O:kO:kO and 2-kO:kO coordination modes to generate a two-dimensional structure (Fig. 2c [Figure 2: see original paper]). Hydrogen bonding and · · · stacking interactions exist between neighboring 2D structures of CP 2, playing a critical role in the formation and stabilization of the three-dimensional supramolecular architecture (Fig. 2d [Figure 2: see original paper]). Geometrical parameters for all hydrogen bonds and ··· stacking interactions are listed in Table 2 .

3.3 IR Spectra

The IR spectra exhibit characteristic absorption bands for water molecules, carboxylate groups, and phenyl rings. As shown in Fig. 3 [Figure 3: see original paper], CPs 1 and 2 display broad absorption bands at 3405 and 3472 cm ^{1}, respectively, corresponding to the O–H stretching frequencies of coordinated water molecules. Strong bands at 1690 and 1677 cm ^{1} represent the characteristic stretching vibrations of carboxylate groups in CPs 1 and 2, respectively. The characteristic phenyl ring bands at 813 and 826 cm ^{1} are attributed to C–H vibrations for 1 and 2, respectively.

3.4 Thermogravimetric Analyses

The thermal analysis curves for 1 and 2 were investigated. For CP 1, the first weight loss of 5.20% observed from 70 to 240 °C corresponds to the release of water molecules (calculated 5.13%). Continued weight loss from 260 to 410 °C is attributed to the departure of ADA^2 and DPE ligands. The final residue of 33.71% is close to the calculated value of 33.00% based on Ag O. For CP 2, the first weight loss of 5.53% below 220 °C results from the loss of water molecules (calculated 5.45%). Above 470 °C, a plateau region is observed, indicating decomposition of the ADA^2 and Bipy ligands, with the final residue being Ag O (found 35.19%, calculated 35.10%).

3.4 Photoluminescence Properties

The fluorescence properties of CPs 1 and 2 were examined in the solid state at room temperature. As shown in Fig. 4 [Figure 4: see original paper], the free H ADA ligand exhibits an intense emission at 415 nm upon excitation at 360 nm, which can be attributed to $\rightarrow n$ *or* $\rightarrow$ transitions. CPs 1 and 2 display maximum emission peaks at 421 and 419 nm as broad bands when excited at 376 and 359 nm, respectively, representing red shifts of 6 and 4 nm relative to the H ADA ligand. However, the emissions of CPs 1 and 2 cannot be attributed to metal-to-ligand or ligand-to-metal charge transfer because the Ag ion has a d^1 configuration and is difficult to oxidize or reduce [24]. Therefore, these emissions may be assigned to intraligand $\rightarrow n$ *or* $\rightarrow$ transitions.

4. Conclusion

Two new coordination polymers, {[Ag(ADA)0.5(DPE)] · H O}n (1) and {[Ag(ADA)0.5(Bipy)0.5] · H O}n (2), have been synthesized by the hydrothermal method, and their structures were determined and characterized by single-crystal X-ray diffraction analysis, elemental analysis, IR spectroscopy, and thermal analysis. The crystal structure of CP 1 is a three-dimensional framework consisting of Ag centers, 6-connected ADA^2 anionic ligands (6-kO,O:kO:kO:kO,O:kO:kO), and 2-connected DPE ligands (2-kO:kO). CP 2 forms a three-dimensional supramolecular structure. The Ag–Ag subunits are bridged to form one-dimensional chains, and adjacent 1D chains are linked by ADA^2 (6-kO,O:kO:kO:kO,O:kO:kO) and Bipy (2-kO:kO) ligands to generate two-dimensional structures. Hydrogen bonding and ··· stacking interactions between neighboring 2D structures play a critical role in forming and stabilizing the three-dimensional supramolecular architecture (Fig. 2d [Figure 2: see original paper]). Furthermore, solid-state photoluminescence measurements demonstrate that CPs 1 and 2 exhibit strong emissions at room temperature.

References

(1) Lee, E. J.; Ju, H. Y.; Kim, S. L.; Park, K. M.; Lee, S. S. Anion-directed coordination networks of a flexible S-Pivot ligand and anion exchange in the solid state. Cryst. Growth Des. 2015, 15, 5427-5436.

(2) Chen, L.; Chen, Q.; Wu, M.; Jiang, F.; Hong, M. Controllable coordination-driven self-assembly: from discrete metallocages to Infinite cage-based frameworks. Acc. Chem. Res. 2015, 48, 201-210.

(3) Huang, C.; Chen, D. M.; Zhu, B. X. Syntheses and crystal structures of Hg(II) and Ag(I) complexes containing 2-acetylpyridine-paminobenzoylhydrazone ligand. Chin. J. Struct. Chem. 2017, 36, 471-477.

(4) Lin, Z. J.; Lu, J.; Hong, M. C.; Cao, R. Metal-organic frameworks based on flexible ligands (FL-MOFs): structures and applications. Chem. Soc. Rev. 2014, 43, 5867-5895.

(5) Chen, C. L.; Zhang, J. Y.; Su, C. Y. Coordination assemblies of metallacyclic, prismatic and tubular molecular architectures based on the non-rigid ligands. Eur. J. norg. Chem. 2007, 19, 2997-3010.

(6) Yue, Q.; Qian, X. B.; Yan, L.; Gao, E. Q. A photoluminescent 8-fold (4+4) interpenetrating diamond network formed through strong hydrogen bonds. Inorg. Chem. Commun. 2008, 11, 1067–1070.

(7) Rowland, C. E.; Belai, N.; Knope, K. E.; Cahill, C. L. Hydrothermal synthesis of disulfide-containing uranyl compounds: in situ ligand synthesis versus direct assembly. Cryst. Growth Des. 2010, 10, 1390-1398.

(8) Wang, X. L.; Qin, C.; Wang, E. B.; Xu, L. Supramolecular self-Assembly of zigzag coordination polymer chains: a fascinating three-dimensional polycatenated network featuring an uneven "density of catenations" and

a three-dimensional porous network. Crystal Growth & Design. 2006, 6, 2061-2065.

(9) Gong, L. L.; Feng, X. F.; Luo, F. Novel azo-metal-organic framework showing a 10-connected bct net, breathing behavior, and unique photoswitching behavior toward CO2. Inorg. Chem. 2015, 54, 11587-11589.

(10) Wang, C. C.; Jing, H. P.; Wang, P. Three silver-based complexes constructed from organic carboxylic acid and 4,4 -bipyridine-like ligands: syntheses, structures and photocatalytic properties. J. Mol. Struct. 2014, 1074, 92-99.

(11) Liu, X. Y.; Cen, P. P.; Zhou, H. L.; Jin, X. Y.; Hu, Q. L.; Ji, Y. Q.; Hu, Q. L.; Ji, Y. Q. A new 3D Cd(II) metal-organic framework with discrete (H2O)6 clusters based on flexible cyclohexane-1,2,4,5-tetracarboxylic acid ligand. Inorg. Chem. Commun. 2015, 53, 11-14.

(12) Yang, J.; Ma, J. F.; Liu, Y. Y.; Batten, S. R. Four-, and six-connected entangled frameworks based on flexible bis(imidazole) ligands and long dicarboxylate anions. CrystEngComm. 2009, 11, 151-159.

(13) Liu, X. Y.; Li, F. F.; Ma, X. H.; Cen, P. P.; Luo, S. C.; Shi, Q.; Ma, S. R.; Wu, Y. W.; Zhang, C. C.; Xu, Z.; Song, W. M.; Xie, G.; Chen, S. P. Coligand modifications fine-tuned the structure and magnetic properties of two triple-bridged azido-Cu(II) chain compounds exhibiting ferromagnetic ordering and slow relaxation. Dalton Trans. 2017, 46, 1207-1217.

(14) Liu, X. Y.; Zhou, H. L.; Cen, P. P.; Jin, X. Y.; Xie, G.; Chen, S. P.; Hu, Q. L. Single-ion-magnet behavior in a two-dimensional coordination polymer constructed from CoII nodes and a pyridylhydrazone derivative. Inorg. Chem. 2015, 54, 8884-8886.

(15) Han, C. B.; Wang, Y. L.; Liu, Q. Y. Crystal structure and magnetic properties of a dinuclear terbium compound Tb2(2-anthc)4(anthc)2(1,10-phen)2. Chin. J. Struct. Chem. 2017, 36,705-710.

(16) Kasuga, N. C.; Sugie, A.; Nomiya, K. Syntheses, structures, and antimicrobial activities of water-soluble silver-oxygen bonding complexes with chiral and racemic camphanic acid (Hca) ligands. Dalton. Trans. 2004, 21, 3732-3740.

(17) Silver, S.; Phung, L. T.; Silver, G. Silver as biocides in burn and wound dressings and bacterial resistance to silver compounds. J. Ind. Microbiol. Biotechnol. 2006, 33, 627-634.

(18) Chen, C. Y.; Cheng, P. Y.; Wu, H. H. Homo- and heterochiral coordination polymers of silver with diaminoc-yclohexane as bridging ligand: trends in alkylbenzoates. Inorg. Chem. 2007, 46, 5691-5699.

(19) Hua, J. A.; Zhao, Y.; Kang, Y. S.; Lu, Y.; Sun, W. Y. Solvent-dependent zinc(II) coordination polymers with mixed ligands: selective sorption and fluorescence sensing. Dalton Trans. 2015, 44, 11524-11532.

(20) Sheldrick, G. M. SADABS. University of Gottingen, Germany 1996.

(21) Sheldrick, G. M. SHELXS-97, Program for Crystal Structure Determination. University of Göttingen, Germany 1997.

(22) Sheldrick, G. M. SHELXL-97, Program for Crystal Structure Refinement, University of Göttingen, Germany 1997.

(23) Hao, H. Q.; Chen, Z. C.; Kuang, W. C.; Peng, M. X. Racemic and homochiral coordination polymers based on carboxylates of different lengths. J. Coord. Chem. 2015, 68, 2715-2724.

(24) Yu, M. H.; Hu, M.; Wu, Z. T. Synthesis, crystal structures and properties of transition metal coordination polymers based on a rigid triazole dicarboxylic acid. RSC Adv. 2013, 3, 25175-25183.

Figure Captions

Fig. 1a. Asymmetric unit of complex 1. Symmetry codes: #1: -x, 2-y, 1-z; #2: 1-x, 2-y, 1-z

Fig. 1b. 2D network of complex 1 in the ac-plane

Fig. 1c. 3D network of complex 1

Fig. 2a. Asymmetric unit of CP 2. Symmetry codes: #1: -x, 1-y, -z; #2: -x, 1-y, -z

Fig. 2b. 1D chain structure of CP 2

Fig. 2c. 2D structure of CP 2

Fig. 2d. 3D structure of CP 2

Fig. 3. IR spectra of CPs 1 and 2

Fig. 4. Solid-state emission spectra of CPs 1 and 2

Tables

Table 1. Selected Bond Lengths (Å) and Bond Angles (°) for CPs 1 and 2

Ag(1)-O(1) Ag(1)-O(2) Angle Dist.

Dist. 2.420(3) Ag(1)-O(1)#1 2.375(3) Ag(1)-O(1)#2 Dist. 2.600(3) 2.738(3) Ag(1)-N(2) 2.243(3) Angle Angle O(1)-Ag(1)-O(1)#2 77.11(10) N(2)-Ag(1)-O(1)#2 91.61(10) O(1)#2-Ag(1)-O(1)#1 99.81(10) O(1)-Ag(1)-O(1)#1 102.72(7) N(2)-Ag(1)-O(1) 137.91(11) O(1)-Ag(1)-O(2) 50.29(9) Dist.

Dist. Ag(1)-O(2)#1 2.234(8) Ag(1)-O(1) 2.241(7) Ag(1)-N(2) Ag(1)-Ag(1)#1 2.892(2) Ag(1)-O(1)#2 2.913(4) Dist. 2.376(9) Angle Angle Angle O(2)#1-Ag(1)-Ag(1)#1 85.2(2) O(1)-Ag(1)-Ag(1)#1 77.5(2) O1(1)#2-Ag(1)-O(2)#1 83.1(3) O(1)#2-Ag(1)-Ag(1)#1 93.5(6) O(1)-Ag(1)-N2 88.9(3) O(2)#1-Ag(1)-N(2) 109.2(3) Symmetry codes of 1: #1: -x, 2-y, 1-z; #2: 1-x, 2-y, 1-z. Symmetry codes of 2: #1: 1-x, 1-y, -z; #2: x, 1-y, -0.5+z

Table 2. Geometrical Parameters of All Hydrogen Bonds and - Interactions for CP 2

D-H· · ·A d(D-H)/Å d(H· · ·A)/Å d (D-H· · ·A)/Å DHA/° O(3)-H(3)· · ·O(2)#1 O(3)-H(3)· · ·O(2)#2 2.905(4) 2.887(4) Cg(i)-Cg(j) Cg(i)-Cg(j) Cg(i)-Perp Cg(j)-Perp - stacking Cg(1)-Cg(2) Cg(3)-Cg(4) Symmetry codes: #1: -3-x, -2-y, -4-z; #2: -3+x, -2-y, -3.5+z. Cg(1, light blue): C(2)C(3)C(4)C(5)C(6)C(7); Cg(2, lightblue): N(2)C(8)C(9)C(10)C(11)C(12); Cg(3, pink): C(2)C(3)C(4)C(5)C(6)C(7); Cg(4, pink): N(2)C(8)C(9)C(10C(11)C(12)

Note: Figure translations are in progress. See original paper for figures.

Source: ChinaXiv —Machine translation. Verify with original.