

## 喹啉和吡啶取代三芳基三唑的两个铜配合物的合成与晶体结构

冯 哲<sup>1</sup> 高健飞<sup>1</sup> 李 刚<sup>1</sup> 朱敦如<sup>\*,1,2</sup>

(<sup>1</sup> 南京工业大学化工学院, 材料化学工程国家重点实验室, 南京 211816)

(<sup>2</sup> 南京大学配位化学国家重点实验室, 南京 210023)

**摘要:** 分别以 3-(2-吡啶基)-4-(4-甲基苯基)-5-(2-喹啉基)-1,2,4-三氮唑(L<sup>1</sup>)和 3-(2-吡啶基)-4-(4-氟苯基)-5-(2-喹啉基)-1,2,4-三氮唑(L<sup>2</sup>)作为配体, 合成了 2 个新的单核铜配合物: *trans*-[Cu(L<sup>1</sup>)<sub>2</sub>(NO<sub>3</sub>)(H<sub>2</sub>O)]NO<sub>3</sub>·H<sub>2</sub>O (**1**)和 *trans*-[Cu(L<sup>2</sup>)<sub>2</sub>(NO<sub>3</sub>)(H<sub>2</sub>O)]NO<sub>3</sub>·H<sub>2</sub>O (**2**), 对其进行了红外、元素分析和单晶结构表征。2 个配合物都属于三斜晶系, *P* $\bar{1}$  空间群。单晶结构表明, 配合物 **1** 和 **2** 中的铜离子均处于一个扭曲的八面体配位环境[CuN<sub>4</sub>O<sub>2</sub>], 轴向上各有一个水分子和一个硝酸根配位。配体的吡啶氮原子和三氮唑的一个氮原子参与配位, 而喹啉的氮原子不配位。配合物晶体中存在 O—H···O、C—H···O、C—H···N 氢键和 C—H··· $\pi$  相互作用, 从而连接单核配合物形成三维网络。

**关键词:** 合成; 铜配合物; 晶体结构; 三芳基三氮唑

中图分类号: O614.121

文献标识码: A

文章编号: 1001-4861(2020)06-1169-07

DOI: 10.11862/CJIC.2020.100

## Syntheses and Crystal Structures of Two Copper Complexes Based on Quinolyl and Pyridyl Substituted Triaryltriazoles

FENG Zhe<sup>1</sup> GAO Jian-Fei<sup>1</sup> LI Gang<sup>1</sup> ZHU Dun-Ru<sup>\*,1,2</sup>

(<sup>1</sup>College of Chemical Engineering, State Key Laboratory of Materials-Oriented Chemical Engineering, Nanjing Tech University, Nanjing 211816, China)

(<sup>2</sup>State Key Laboratory of Coordination Chemistry, Nanjing University, Nanjing 210023, China)

**Abstract:** Two new copper(II) complexes, *trans*-[Cu(L<sup>1</sup>)<sub>2</sub>(NO<sub>3</sub>)(H<sub>2</sub>O)]NO<sub>3</sub>·H<sub>2</sub>O (**1**) and *trans*-[Cu(L<sup>2</sup>)<sub>2</sub>(NO<sub>3</sub>)(H<sub>2</sub>O)]NO<sub>3</sub>·H<sub>2</sub>O (**2**) (L<sup>1</sup>=3-(2-pyridyl)-4-(*p*-methylphenyl)-5-(2-quinolyl)-1,2,4-triazole, L<sup>2</sup>=3-(2-pyridyl)-4-(*p*-fluorophenyl)-5-(2-quinolyl)-1,2,4-triazole), were synthesized and characterized by FT-IR, elemental analyses and single-crystal X-ray crystallography. Both **1** and **2** crystallize in triclinic system with space group *P* $\bar{1}$ . X-ray crystallography analysis reveals that the copper ion in **1** and **2** lies in a distorted octahedral environment [CuN<sub>4</sub>O<sub>2</sub>] with one nitrate and one water molecule, respectively in the *trans*-position. The L<sup>1</sup> or L<sup>2</sup> ligand coordinates with Cu(II) via one pyridine N atom and one triazole N atom, while the quinolyl group does not take part in coordination. In **1** and **2** there are some intermolecular O—H···O, C—H···O and C—H···N hydrogen bonds and C—H··· $\pi$  interactions, connecting the mononuclear complexes to form a 3D framework. CCDC: 1975981, **1**; 1975982, **2**.

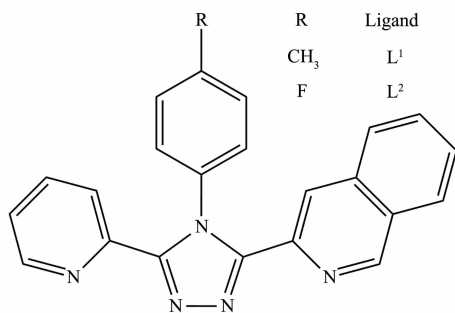
**Keywords:** synthesis; Cu(II) complex; crystal structure; triaryltriazole

收稿日期: 2020-01-22。收修改稿日期: 2020-03-07。

江苏省自然科学基金(No.BK20181374)和南京大学配位化学国家重点实验室开放课题资助项目。

\*通信联系人。E-mail: zhudr@njtech.edu.cn; 会员登记号: S060015982P。

3,4,5-Triarylsubstituted 1,2,4-triazole is a kind of very useful ligand in coordination chemistry due to its rich and versatile coordination modes<sup>[1-2]</sup>. Specially, some iron(II) complexes based on the triaryltriazole can show interesting spin-crossover properties<sup>[3]</sup>, which makes them be a type of potential molecular-based materials used as memory devices, displays and switching<sup>[4-5]</sup>. In order to explore novel triaryltriazole-based iron(II) spin-crossover complexes, a series of 4-aryl-substituted 3,5-di(2-pyridyl)-1,2,4-triazoles<sup>[6-12]</sup> and asymmetrically 3,4,5-triarylsubstituted 1,2,4-triazoles<sup>[13-25]</sup> have been designed and synthesized successfully. Among them, the pyridyl, phenyl, pyrrolyl, imidazolyl and benzimidazolyl groups are the known aromatic rings attached on the 3,4,5-triarylsubstituted 1,2,4-triazoles. However, the quinolyl group, an important alkaloid with stronger conjugated system, is less observed to connect on the 1,2,4-triazoles. Up to now only two quinolyl substituted 1,2,4-triazoles have been reported by us<sup>[26-27]</sup>. As a continuation of our investigation of the quinolyl substituted 1,2,4-triazoles, we designed and synthesized two new triaryltriazoles: 3-(2-pyridyl)-4-(*p*-methylphenyl)-5-(2-quinolyl)-1, 2, 4-triazole (**L**<sup>1</sup>) and 3-(2-pyridyl)-4-(*p*-fluorophenyl)-5-(2-quinolyl)-1,2,4-triazole (**L**<sup>2</sup>) as shown in Scheme 1. Herein we present the syntheses, crystal structures and spectral characterization of two copper (II) complexes based on these ligands: *trans*-[Cu(**L**<sup>1</sup>)<sub>2</sub>(NO<sub>3</sub>)(H<sub>2</sub>O)]NO<sub>3</sub>·H<sub>2</sub>O (**1**) and *trans*-[Cu(**L**<sup>2</sup>)<sub>2</sub>(NO<sub>3</sub>)(H<sub>2</sub>O)]NO<sub>3</sub>·H<sub>2</sub>O (**2**).



Scheme 1 Structures of the ligands **L**<sup>1</sup> and **L**<sup>2</sup>

## 1 Experimental

### 1.1 Materials and measurements

All chemicals used were of analytical grade.

Solvents were purified by conventional methods. The ligands **L**<sup>1</sup> and **L**<sup>2</sup> were synthesized via a similar literature method<sup>[23]</sup>. Elemental analyses (C, H, N) were carried out with a Thermo Finnigan Flash 1112A elemental analyzer. IR spectra were recorded on a Nicolet Avatar 380 FT-IR instrument with KBr pellets in a range of 4 000~400 cm<sup>-1</sup>.

### 1.2 Syntheses of complexes **1** and **2**

A solution of Cu(NO<sub>3</sub>)<sub>2</sub>·3H<sub>2</sub>O (0.05 mmol) in MeOH (3 mL) was added to a solution of **L**<sup>1</sup> (0.1 mmol) in anhydrous MeOH (3 mL). The mixture was stirred for 4 h at room temperature. A resulting green product was filtered and washed with H<sub>2</sub>O, then dried under vacuum to give 0.042 mmol (84%) of complex **1**. The green single crystals of **1** suitable for X-ray diffraction were obtained by slow evaporation from the MeOH/MeCN (1:1, V/V) solution of the complex. Elemental analyses Calcd. for C<sub>46</sub>H<sub>38</sub>CuN<sub>12</sub>O<sub>8</sub>(%): C, 58.13; H, 4.03; N, 17.69. Found(%): C, 57.81; H, 4.25; N, 17.46. IR (KBr, cm<sup>-1</sup>): 3 343(w), 3 049(w), 3 011(w), 2 918(w), 1 597(m), 1 498(s), 1 387(vs), 1 289(m), 1 086(w), 828(m), 761(m).

The prepared procedure for **2** was the same as that for **1** except using **L**<sup>2</sup> (0.1 mmol) to replace **L**<sup>1</sup>. Yield: 86.2%. Elemental analyses Calcd. for C<sub>44</sub>H<sub>32</sub>CuF<sub>2</sub>N<sub>12</sub>O<sub>8</sub>(%): C, 55.14; H, 3.37; N, 17.54. Found(%): C, 55.31; H, 3.26; N, 17.69. IR (KBr, cm<sup>-1</sup>): 3 379(w), 3 075(w), 1 596(m), 1 508(vs), 1 384(s), 1 236(m), 1 155(w), 839(m), 759(m).

### 1.3 Crystal structure determination

The well-shaped single crystals of **1** and **2** were selected for X-ray diffraction study. The unit cell parameters and intensity data were collected at 296(2) K on a Bruker SMART APEX II CCD diffractometer using a graphite-monochromated Mo K $\alpha$  ( $\lambda$ =0.071 073 nm) radiation. The structures were solved by direct methods and refined on *F*<sup>2</sup> by full-matrix least squares procedures using SHELXTL software<sup>[28]</sup>. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were fixed in calculated positions and refined isotropically. Two NO<sub>3</sub><sup>-</sup> anions, O1W and O2W were found to be highly disordered with an occupancy factor of 0.5. Due to the disorder, the hydrogen atoms

on the water were not calculated. The crystallographic data of **1** and **2** are listed in Table 1, and the selected bond lengths and angles are provided in Table 2. CCDC: 1975981, **1**; 1975982, **2**.

**Table 1** Crystal data and structure refinement for **1** and **2**

Complex	<b>1</b>	<b>2</b>
Empirical formula	C <sub>46</sub> H <sub>38</sub> CuN <sub>12</sub> O <sub>8</sub>	C <sub>44</sub> H <sub>32</sub> CuF <sub>2</sub> N <sub>12</sub> O <sub>8</sub>
Formula weight	950.42	958.36
Crystal system	Triclinic	Triclinic
Space group	$P\bar{1}$	$P\bar{1}$
<i>a</i> / nm	0.854 51(5)	0.841 6(4)
<i>b</i> / nm	0.961 20(7)	0.958 7(4)
<i>c</i> / nm	1.485 7(3)	1.448 2(6)
$\alpha$ / (°)	96.812(3)	100.209(6)
$\beta$ / (°)	106.423(3)	103.144(6)
$\gamma$ / (°)	101.713(2)	100.201(6)
<i>V</i> / nm <sup>3</sup>	1.125 8(4)	1.090 6(8)
<i>Z</i>	1	1
<i>D<sub>c</sub></i> / (g·cm <sup>-3</sup> )	1.402	1.459
$\mu$ / mm <sup>-1</sup>	0.553	0.578
<i>F</i> (000)	491	491
Crystal size / mm	0.13×0.11×0.07	0.16×0.12×0.08
$\theta$ range / (°)	1.45~25.00	1.48~25.00
Reflection collected	8 196	7 766
Independent reflection	3 943 ( <i>R</i> <sub>int</sub> =0.037 4)	3 784 ( <i>R</i> <sub>int</sub> =0.023 1)
Reflection observed [ <i>I</i> >2 $\sigma$ ( <i>I</i> )]	2 478	3 006
Data, restraint, parameter	3 943, 96, 351	3 784, 114, 352
Goodness-of-fit on <i>F</i> <sup>2</sup>	1.025	1.118
<i>R</i> <sub>1</sub> , <i>wR</i> <sub>2</sub> [ <i>I</i> >2 $\sigma$ ( <i>I</i> )]	0.069 8, 0.187 9	0.056 1, 0.170 4
<i>R</i> <sub>1</sub> , <i>wR</i> <sub>2</sub> (all data)	0.115 1, 0.207 9	0.070 6, 0.181 8
( $\Delta\rho$ ) <sub>max</sub> , ( $\Delta\rho$ ) <sub>min</sub> / (e·nm <sup>-3</sup> )	725, -345	547, -396

**Table 2** Selected bond distances (nm) and bond angles (°) for **1** and **2**

<b>1</b>					
Cu1-N1	0.203 3(3)	Cu1-N2	0.197 0(4)	Cu1-O1	0.269 7(2)
Cu1-O1W	0.239 7(19)	N2-N3	0.136 1(5)	C20-C23	0.151 6(6)
N1-Cu1-N2	80.31(14)	N1-Cu1-O1	96.76(2)	N2-Cu1-O1	96.95(2)
N1-Cu1-O1W	94.9(3)	O1-Cu1-O1W <sup>i</sup>	170.4(3)		
<b>2</b>					
Cu1-N1	0.203 6(3)	Cu1-N2	0.197 9(3)	Cu1-O1	0.263 9(3)
Cu1-O1W	0.247 5(3)	N2-N3	0.136 2(4)	C20-F1	0.136 4(4)
N1-Cu1-N2	80.33(12)	N1-Cu1-O1	95.20(2)	N2-Cu1-O1	93.78(2)
N1-Cu1-O1W	94.87(2)	O1-Cu1-O1W <sup>i</sup>	174.9(3)		

Symmetry code: <sup>i</sup> -*x*, -*y*, -*z* for **1**; <sup>i</sup> 1-*x*, 1-*y*, 1-*z* for **2**.

## 2 Results and discussion

### 2.1 Synthesis

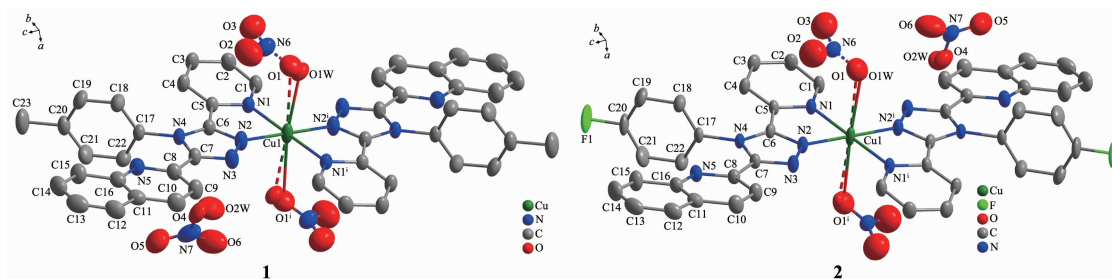
Asymmetrically quinolyl substituted 3,4,5-triaryl-1,2,4-triazoles ( $L^1$  and  $L^2$ ) react with  $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$  in molar ratio of 2:1 to form two monomeric complexes, *trans*- $[\text{Cu}(L^1)_2(\text{NO}_3)(\text{H}_2\text{O})]\text{NO}_3 \cdot \text{H}_2\text{O}$  (**1**) and *trans*- $[\text{Cu}(L^2)_2(\text{NO}_3)(\text{H}_2\text{O})]\text{NO}_3 \cdot \text{H}_2\text{O}$  (**2**), which are stable in air. The yields for **1** and **2** are 84% and 86.2%, respectively. The elemental analyses were satisfactory and indicate that both **1** and **2** contain one Cu(II), two triazole ligands, two  $\text{NO}_3^-$  and two water molecules.

### 2.2 Crystal structures of **1** and **2**

The crystal structures of **1** and **2** are presented in Fig.1 together with the atomic labeling system. Complexes **1** and **2** all crystallize in the triclinic space group  $P\bar{1}$  and there is an inversion center at the Cu(II) ion. Because **1** and **2** are isostructural complexes, herein, only the structure of **1** is discussed in detail. The asymmetric unit of **1** consists of half Cu(II) cation, one  $L^1$  ligand, one coordinated  $\text{NO}_3^-$  and  $\text{H}_2\text{O}$  molecule (their occupancy factors are 0.5), one  $\text{NO}_3^-$  counter ion and one lattice  $\text{H}_2\text{O}$  molecule (their occupancy factors are also 0.5), which is agreement with the elemental analysis result. The Cu(II) ion of **1** is coordinated by four nitrogen atoms from two  $L^1$  ligands in the equatorial plane and two oxygen atoms from  $\text{NO}_3^-$  and  $\text{H}_2\text{O}$  in the axial positions to form a distorted octahedral  $[\text{CuN}_4\text{O}_2]$  geometry. Each  $L^1$  ligand coordinates to Cu(II) ion via N1 atom of the pyridyl and N2 atom of the triazole, similar to the coordination modes in some related Cu(II) complexes<sup>[13,15,17,29-30]</sup>. The quinolyl group of  $L^1$  ligand is uncoordinated, which is different from

the Fe(II) complex with quinolyl substituted triaryl-triazole: *cis*- $[\text{FeL}_2(\text{NCS})_2]$  ( $L=3-(p\text{-methylphenyl})\text{-4-phenyl-5-(2-quinolyl)-1,2,4-triazole}$ )<sup>[27]</sup>. The distance of Cu1-O1 (0.269 7 nm) is longer than the Cu1-O1W one (0.239 7 nm). The Cu-N bond lengths are within the normal ranges observed for the octahedral Cu(II) complexes<sup>[13,15,17,29-30]</sup>. However, the Cu-N bond to the triazole nitrogen is 0.006 3 nm shorter than that to the pyridyl nitrogen. The same feature has been observed in the similar Cu(II) complexes<sup>[13,15,17]</sup>. The ligand  $L^1$  in **1** is non-planar. The triazole makes dihedral angles of  $4.8(3)^\circ$ ,  $10.1(3)^\circ$  and  $83.3(3)^\circ$  with the quinolyl ring, the pyridyl ring and *p*-methylphenyl ring, respectively. The corresponding angles in  $L^2$  of **2** are  $8.7(3)^\circ$ ,  $9.0(3)^\circ$  and  $86.8(3)^\circ$ , respectively.

There are many intermolecular hydrogen bonds interactions in **1** (Fig.2, Table 3), associated with the closer crystal packing. These hydrogen bond interactions include: (1) between water molecules and  $\text{NO}_3^-$  anion ( $\text{O1W} \cdots \text{O4}$  and  $\text{O2W}^i \cdots \text{O1}^i$ ); (2) between pyridyl group and triazole ring ( $\text{C1-H1A} \cdots \text{N3}^i$ ); (3) between pyridyl and  $\text{NO}_3^-$  anion ( $\text{C2-H2A} \cdots \text{O3}^{ii}$  and  $\text{C3-H3A} \cdots \text{O4}^{ii}$ ); (4) between quinolyl group and the coordinated  $\text{NO}_3^-$  ( $\text{C10-H10A} \cdots \text{O2}^{iii}$  and  $\text{C12-H12A} \cdots \text{O1}^{iii}$ ); (5) between *p*-methylphenyl ring and the uncoordinated  $\text{NO}_3^-$  ( $\text{C22-H22A} \cdots \text{O4}$ ). In addition, there are an intramolecular edge-to-face C-H  $\cdots \pi$  interaction involving C4-H4A and *p*-methylphenyl ring ( $\text{H4A} \cdots \pi$  0.294 nm and  $\angle \text{C4-H4A} \cdots \pi = 145^\circ$ ) and an intermolecular edge-to-face C-H  $\cdots \pi$  interaction involving C19-H19A and the phenyl ring of quinolyl group ( $\text{H19A} \cdots \pi$  0.326 nm and  $\angle \text{C19-H19A} \cdots \pi = 141^\circ$ ) (Table 3, Fig.2). Notably, in **1** an offset face-to-

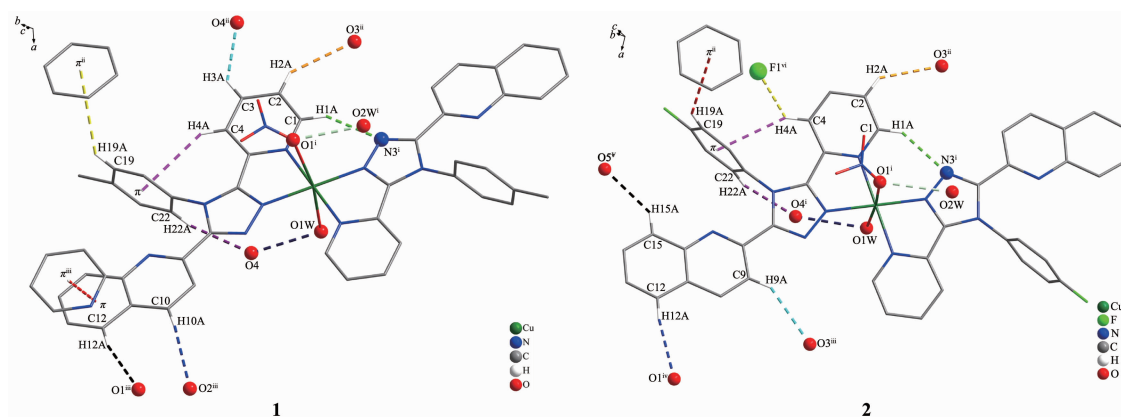


All H atoms are omitted for clarity; Symmetry code:  $^i -x, -y, -z$  for **1**;  $^i 1-x, 1-y, 1-z$  for **2**

Fig.1 Projection of structures of **1** and **2** with 30% thermal ellipsoids probability

face  $\pi$ - $\pi$  stacking interaction exists between the phenyl ring of quinolyl group and pyridyl ring (dihedral angle:  $12.2(3)^\circ$ ) with a centroid-centroid distance of 0.382 nm (Fig.2, Table 4), while the corresponding stacking is

not found in **2**. These extensive hydrogen bonds and C-H $\cdots\pi$  interactions assemble the mononuclear units,  $\text{NO}_3^-$  anions and lattice water molecule into a 3D framework of the complexes (Fig.3).



Symmetry codes: <sup>i</sup>  $-x, -y, -z$ ; <sup>ii</sup>  $x-1, y, z$ ; <sup>iii</sup>  $1+x, 1+y, z$  for **1**; <sup>i</sup>  $1-x, 1-y, 1-z$ ; <sup>ii</sup>  $x-1, y, z$ ; <sup>iii</sup>  $2-x, 1-y, 1-z$ ; <sup>iv</sup>  $1+x, 1+y, z$ ; <sup>v</sup>  $1+x, 1+y, 1+z$  for **2**

Fig.2 Hydrogen-bonding, C-H $\cdots\pi$  and  $\pi\cdots\pi$  interactions in **1** and **2**

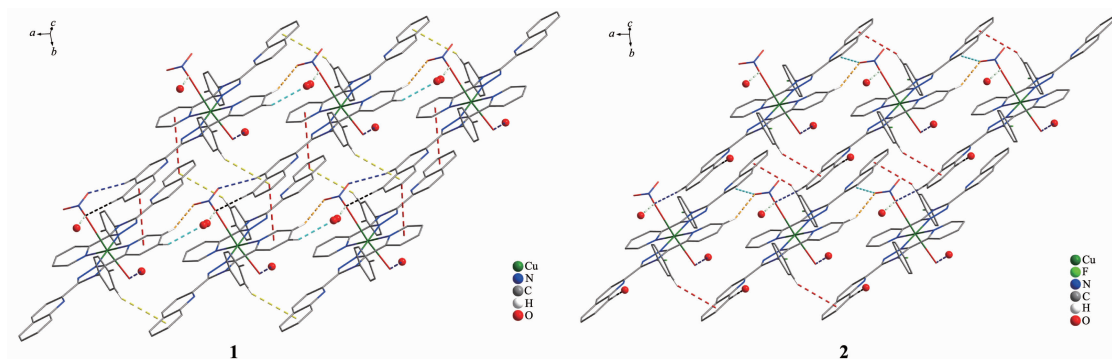
Table 3 Hydrogen-bond geometry and C-H $\cdots\pi$  interactions in **1** and **2**

D-H $\cdots$ A	$d(\text{D-H}) / \text{nm}$	$d(\text{H}\cdots\text{A}) / \text{nm}$	$d(\text{D}\cdots\text{A}) / \text{nm}$	$\angle \text{D-H}\cdots\text{A} / (^\circ)$
<b>1</b>				
C1-H1A $\cdots$ N3 <sup>i</sup>	0.093	0.233	0.313 8(2)	144
C2-H2A $\cdots$ O3 <sup>ii</sup>	0.093	0.263	0.341 9(2)	143
C3-H3A $\cdots$ O4 <sup>ii</sup>	0.093	0.264	0.338 0(2)	137
C4-H4A $\cdots\pi(\text{Ph})$	0.093	0.294	0.373 8(4)	145
C10-H10A $\cdots$ O2 <sup>iii</sup>	0.093	0.271	0.361 8(2)	167
C12-H12A $\cdots$ O1 <sup>iii</sup>	0.093	0.269	0.360 6(2)	166
C19-H19A $\cdots\pi(\text{Ph})$ <sup>ii</sup>	0.093	0.326	0.402 4(4)	141
C22-H22A $\cdots$ O4	0.093	0.261	0.327 2(2)	153
O1W $\cdots$ O4	—	—	0.278 5(2)	—
O2W <sup>iv</sup> $\cdots$ O1 <sup>i</sup>	—	—	0.265 8(2)	—
<b>2</b>				
C1-H1A $\cdots$ N3 <sup>i</sup>	0.093	0.234	0.314 1(2)	144
C2-H2A $\cdots$ O3 <sup>ii</sup>	0.093	0.259	0.335 5(2)	139
C4-H4A $\cdots\pi(\text{Ph})$	0.093	0.291	0.373 3(4)	147
C4-H4A $\cdots$ F <sup>vi</sup>	0.093	0.260	0.311 4(2)	116
C9-H9A $\cdots$ O3 <sup>iii</sup>	0.093	0.267	0.349 4(2)	147
C12-H12A $\cdots$ O1 <sup>iv</sup>	0.093	0.257	0.349 2(2)	170
C15-H15A $\cdots$ O5 <sup>v</sup>	0.093	0.261	0.340 1(2)	143
C19-H19A $\cdots\pi(\text{Ph})$ <sup>ii</sup>	0.093	0.301	0.377 5(4)	141
C22-H22A $\cdots$ O4 <sup>i</sup>	0.093	0.243	0.326 3(3)	148
O1W $\cdots$ O2W <sup>i</sup>	—	—	0.266 2(3)	—
O2W $\cdots$ O1 <sup>i</sup>	—	—	0.283 9(3)	—

Symmetry codes: <sup>i</sup>  $-x, -y, -z$ ; <sup>ii</sup>  $x-1, y, z$ ; <sup>iii</sup>  $1+x, 1+y, z$  for **1**; <sup>i</sup>  $1-x, 1-y, 1-z$ ; <sup>ii</sup>  $x-1, y, z$ ; <sup>iii</sup>  $2-x, 1-y, 1-z$ ; <sup>iv</sup>  $1+x, 1+y, z$ ; <sup>v</sup>  $1+x, 1+y, 1+z$ ; <sup>vi</sup>  $1-x, 2-y, 2-z$  for **2**.

Table 4  $\pi \cdots \pi$  interaction in **1**

$\pi \cdots \pi$ interaction	$d(\text{cent} \cdots \text{cent}) / \text{nm}$	Dihedral angle / ( $^\circ$ )
$\pi(\text{Ph}) \cdots \pi(\text{Py})^{\text{iii}}$	0.382	12.2(3)

Symmetry code: <sup>iii</sup>  $1+x, 1+y, z$ .Fig.3 Three-dimensional frameworks of **1** and **2**

### 2.3 IR spectra

In the IR spectra of complexes **1** and **2**, a weak broad peak at  $3\,343\text{ cm}^{-1}$  (**1**) or  $3\,379\text{ cm}^{-1}$  (**2**) can be attributed to the O-H stretching vibrations of water molecules. A medium band at  $1\,597\text{ cm}^{-1}$  (**1**) or  $1\,596\text{ cm}^{-1}$  (**2**) can be assigned to the coordinated pyridyl ring vibration<sup>[14]</sup>. A strong band at  $1\,384\text{ cm}^{-1}$  is assigned to characteristic N=O stretching vibrations of  $\text{NO}_3^-$  in **1** and **2**<sup>[31]</sup>. In addition, the stretching vibration of F-C(Ph) in **2** can be observed at  $1\,236\text{ cm}^{-1}$ <sup>[32]</sup>. These features are in consistent with the results of the X-ray analysis.

### 3 Conclusions

Two new Cu(II) complexes based on the quinolyl and pyridyl substituted triaryltriazole have been synthesized and characterized by IR and X-ray crystallography. Structural analyses indicate that two complexes have a similar distorted octahedral  $[\text{CuN}_4\text{O}_2]$  core with one nitrate and one water molecule, respectively in the *trans*-position.

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