Synthesis, crystal structure, photoluminescent and antimicrobial properties of a thiocyanato-bridged copper(II) coordination polymer

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Synthesis, crystal structure, photoluminescent and antimicrobial properties of a thiocyanato-bridged copper(II) coordination polymer

Feudjio Tsague Chimaine1, Divine Mbom Yufanyi2, Amah Colette Benedicta Yuoh1, Donatus Bekindaka Eni1 and Moise Ondoh Agwara1*

Abstract: A Cu(II) 1D polymer with mixed ligands (SCN− and pyridine) has been synthesized and characterized by elemental analyses, IR, UV–visible and TG-DTA analytical techniques. The crystal structure was determined by single-crystal X-ray diffraction analyses. The complex crystallizes in the triclinic crystal system with space group \( \text{P} \bar{1} \) with one formula unit. Each Cu(II) atom is six coordinate with two N atoms of two pyridine molecules, two N atoms and two S-atoms from bridging SCN anions giving a distorted octahedral geometry with a CuS2N4 chromophore. The spectroscopic, photoluminescent and the antimicrobial activities of the synthesized complex were investigated.

Keywords: crystal structure; copper(II); photoluminescence; antimicrobial properties; thiocyanate

1. Introduction

Research interest in coordination polymers has increased recently not only as a result of their fascinating topologies and intriguing frameworks but also due to their potential applications in gas storage, separation, biosensing, luminescence, magnetism, conductivity, nanoparticles, antimicrobial...
activity and catalysis (Batten, Harris, Murray, & Smith, 2002; Eddaoudi et al., 2001; Etaiw & El-bendary, 2013; Henninger, Jeremias, Kummer, & Janiak, 2012; Janiak, 2003; Rowsell & Yaghi, 2004; Zaworotko, 2001). The topology and dimensionality of these frameworks is dependent on the rational choice of the metal ion and the ligands. Weak intermolecular interactions such as hydrogen bonding and π–π stacking interactions may also play an important role on the overall arrangement and influence the properties (Baca et al., 2008; Batten et al., 2002; Prins, Reinholdt, & Timmerman, 2001; Whitesides & Boncheva, 2002). Furthermore, synthesis conditions (synthetic methods, reaction temperature, metal/ligand ratio, pH value and the types of solvents) can also greatly influence the crystal structure and its dimensionality (Etaiw & El-bendary, 2013).

The design and synthesis of one-dimensional coordination polymers is important since they can be used as examples for developing theoretical models of the exchange interaction in extended lattices (Demir, Yilmaz, Sariboga, Buyukgungor, & Mrozinski, 2010). Choice of organic ligands and metal ions is of great importance in the construction of these polymeric structures. Transition metals show rich diversity of oxidation states, coordination numbers and geometries, and their complexes and solid-state compounds possess an array of interesting redox, magnetic, optical, electrical and catalytic properties (Chattopadhyay et al., 2012; Chattopadhyay, Drew, Diaz, & Ghosh, 2007; Demir et al., 2010; Hong, 2008; Hu, Li, Wang, Du, & Guo, 2009).

Among several ligands employed, SCN− is a highly versatile ambidentate ligand with two different donor atoms, which can coordinate through terminal modes or bridging modes: end-to-end (μ-1,3-NCS) and end-on (μ-1,1-NCS, μ-1,1-SCN) fashions via the nitrogen and sulphur atoms to generate coordination networks as well as interlink the one- or two-dimensional molecules into frameworks via non-covalent interactions (Li, Liang, & Tian, 2011; Shen & Feng, 2002). The rational design and construction of thiocyanato-brigded coordination polymers has been explored due to their fascinating topologies and remarkable properties (Bai, Shang, Dang, Sun, & Gao, 2009; Banerjee, Drew, & Ghosh, 2003; Chattopadhyay et al., 2007, 2012; Das et al., 2012; Hong, 2008; Li et al., 2011; Shi et al., 2005; You & Zhu, 2005; Yue et al., 2008). The thiocyanate group plays a key role in stabilizing a variety of transition metal centres and determining the structure of polymeric transition-metal complexes (Das et al., 2012). Recently, a large number of thiocyanato-bridged coordination polymers with intriguing topologies and fascinating properties have been reported (Bai et al., 2009; Banerjee et al., 2003; Chattopadhyay et al., 2007, 2012; Das et al., 2012; Li et al., 2011; Neumann, Jess, & Näther, 2014; Shen & Feng, 2002; Shi et al., 2005; You & Zhu, 2005; Yue et al., 2008). Among these are the thiocyanato-bridged copper(II) coordination polymers with N-donor auxiliary ligands (Das et al., 2012; Hong, 2008; Shen & Feng, 2002; Shi et al., 2005).

However, controlled synthesis of coordination polymers with preferred structures is still a challenge. Self-assembly of these coordination polymers through a mixed ligand strategy has progressively become an effective approach, which is expected to generate frameworks with more diverse structural motifs (Du, Li, Liu, & Fang, 2013; Shirdel, Marandi, Jalilzadeh, Huber, & Pfitzner, 2015; Yang & Sun, 2013). Auxiliary ligands such as N-donor heterocyclic ligands play a significant role in many biological systems, being a component of several vitamins and drugs (Dhaveethu & Ramachandramoorthy, 2013). Nitrogen-containing heterocycles have been found to possess diverse pharmacological activities (Forood, Flatt, Chassaing, & Katritzky, 2002). Among this group of heterocycles are pyridine and its derivatives. Taking advantage of the coordination ability and properties of copper, pyridine and SCN, herein we report the synthesis, crystal structure and the luminescent properties of a thiocyanate-bridged copper(II) coordination polymer with pyridine. In addition, the in vitro antimicrobial activity of the complex against selected micro-organisms is reported.
2. Experimental

All chemicals and solvents were obtained from commercial sources and were used as received.

2.1. Synthesis of the complex

A 40 mL dry methanolic solution of CuCl₂·2H₂O (5.1144 g; 30 mmol) was poured into a three-neck round bottom flask under nitrogen atmosphere. To this solution was added drop wise, while stirring, a dry methanolic solution of a mixture of NH₄SCN (4.5672 g; 60 mmol) and pyridine (9.617 mL; 120 mmol). Upon addition of the mixed ligand solution into the dark green solution in the round bottom flask, a light green precipitate was formed. The mixture was refluxed for 3 h under nitrogen atmosphere at 30°C. The light green precipitate was filtered, washed with dry methanol, air dried and weighed. The powder was recrystallized by the diffusion method. It was dissolved in DMSO in a small vial and placed in a bigger vial containing DMF (in which it is insoluble). Shiny blue crystals, in good yield (92%), were afforded within 48 h.

2.2. Characterization techniques

The melting point was recorded using a Stuart SMP10 system. Conductivity measurement was carried out in distilled water using a HANNA multimeter H19811-5; pH/°C/EC/TDS meter at room temperature. Elemental analysis (C, H, N, S, Cu) was carried out on a Perkin-Elmer automated model 2400 series II CHNS/M analyser. The infrared spectrum was recorded using a Thermo Scientific Nicolet i55 instrument directly on a small sample of the complex in the range of 400–4,000 cm⁻¹. The UV–vis spectrum of a DMSO solution of the complex was recorded using a Varian, Cary 50 UV–vis spectrophotometer at room temperature. Photoluminescence studies were carried out using a Perkin-Elmer, LS55 Luminescence Spectrometer, while thermal studies were carried out using the TGA/DSC 1 (STAR System) instrument. The TGA analyses were conducted between 30 and 600°C under nitrogen atmosphere at a flow rate of 10 mL min⁻¹ and a temperature ramp of 10°C min⁻¹.

2.3. Single-crystal X-ray structure determination

Intensity data for the compound were collected using a Bruker AXS Kappa APEX II single crystal CCD diffractometer, equipped with graphite-monochromated CuKa radiation (λ = 1.5418 Å) at room temperature. The selected crystal for the diffraction experiment had a dimension of 0.21 × 0.12 × 0.06 mm³. The structure was solved by direct methods and refined by full-matrix least squares (Sheldrick, 1997) on F. The non-hydrogen atoms were refined anisotropically. H atoms were included in calculated positions with C–H lengths of 0.95(CH), 0.99(CH₂) and 0.98(CH₃) Å; Uₚ(C) values were fixed at 1.2Uₚ(C) except for CH₃ where it was 1.5Uₚ(C). They were assigned isotopic thermal parameters and allowed to ride on their parent carbon atoms. All calculations were carried out using the SHELXTL package (Bruker, 2001).

2.4. Antimicrobial tests

The antimicrobial tests were carried out in the laboratory of Phytobiochemical and Medicinal Plant Study, University of Yaounde I. The tests were done on eight pathogenic micro-organisms, 4 yeasts, Candida albicans ATCC P37039, C. albicans 194B, Candida glabrata 44B and Cryptococcus neoformans and 4 bacterial strains, Gram-positive Staphylococcus aureus CIP 7625 and Gram-negatives, Pseudomonas aeruginosa CIP 76110, Salmonella typhi and Escherichia coli ATCC25922 obtained from Centre Pasteur, Yaounde, Cameroon. Reference antibacterial drug chloramphenicol and antifungal drug nystatin were evaluated for their antibacterial and antifungal activities and their results were compared with those of the free ligands and the complex. The disc diffusion method, using Muller Hinton Agar, from the protocol described by the National Committee for Clinical Laboratory Standard was used for preliminary screening. Mueller-Hinton agar was prepared from a commercially available dehydrated base according to the manufacturer’s instructions. Several colonies of each micro-organism were collected and suspended in saline (0.9% NaCl). Then, the turbidity of the test suspension was standardized to match that of a 0.5 McFarland standard (corresponds to approximately 1.5 × 10⁸ CFU/mL for bacteria or 1 × 10⁶ to 5 × 10⁶ cells/mL for yeast). Each compound or reference was accurately weighed and dissolved in the appropriate diluents (DMSO at 10%, methanol at 10%, or distilled water) to yield the required concentration (2 mg mL⁻¹ for compound or 1 mg mL for reference drug), using sterile glassware.
Whatman filter paper number 1 was used to prepare discs approximately 6 mm in diameter, which were packed up with aluminium paper and sterilized by autoclaving. Then, 25 μL of stock solutions of compound or positive control was delivered to each disc, leading to 50 μg of compound or 25 μg of reference drug. The dried surface of a Muller-Hinton agar plate was inoculated by flooding over the entire sterile agar surface with 500 μL of inoculum suspensions. The lid was left ajar for 3 to 5 min to allow for any excess surface moisture to be absorbed before applying the drug-impregnated discs. Discs containing the compounds or antimicrobial agents were applied within 15 min of inoculating the MHA plate. Six discs per Petri dish were plated. The plates were inverted and placed in an incubator set to 35°C. After 18 h (for bacteria) and 24 h (for yeasts) of incubation, each plate was examined. The diameters of the zones of complete inhibition (as judged by the unaided eye) were measured, including the diameter of the disc. Zones were measured to the nearest whole millimetre, using sliding callipers, which were held on the back of the inverted Petri plate. All experiments were carried out in duplicate. The compound was considered active against a microbe if the inhibition zone was 6 mm and above.

3. Results and discussion

3.1. Synthesis of the complex

The title complex was green in colour and air stable, with a sharp melting point (186°C) indicating its purity. The molar conductivity value of 60 Ω cm⁻² mol⁻¹ for the complex in water indicates that it is a nonelectrolyte. The complex was obtained in good yield (92%). The physicochemical properties of the title complex are summarized in Table 1.

3.2. X-ray crystal structure

The ORTEP representation of the asymmetric unit of \([\text{Cu(py)}_2(\text{SCN})_2]_n\) is shown in Figure 1, the unit cell structure in Figure 2, while the 1-D polymeric chain structure together with the atomic numbering

| Table 1. Physical data of the complexes |
|---------------------------------------|
| Complex | Nature | Colour | Yield (%) | Melting point (°C) | Molar conductivity (Ω⁻¹cm² mol⁻¹) | Elemental analyses: %found (%calc.) |
|---------|--------|--------|-----------|-------------------|------------------------------------|----------------------------------|
| \([\text{Cu(py)}_2(\text{SCN})_2]_n\) | Crystals | Green | 92 | 186 | 60 | 40.88 | 3.36 | 16.27 | 19.18 |
|         |        |        |           |                   |                                   | (42.65) | (2.98) | (16.58) | (18.81) |

Figure 1. Asymmetric unit of the complex.
The crystal packing diagram of [Cu(py)$_2$(SCN)$_2$]$_n$ is shown in Figure 4. The crystal data and structure refinement are presented in Table 2, while the selected bond lengths and bond angles are shown in Table 3.
The title compound is a one-dimensional thiocyanato-bridged polymeric structure. The complex crystallizes in the triclinic crystal system with space group \textit{P\overline{1}} and its asymmetric unit (Figure 1) consists of two crystallographically independent copper(II) atoms, of which one (Cu1) is located on a general position whereas the second (Cu2) is located on a crystallographic inversion centre. The structure is polymorphic to \([\text{Cu(Py)}_2(\text{SCN})_2]_n\) (Chen, Bai, & Qu, 2005) and iso-structural with \([\text{Ni(NCS)}_2(\text{pyridine})_2]_n\) (Neumann et al., 2014) found in the literature. There is one molecule in the triclinic unit cell as opposed to three in the previous report (Chen et al., 2005).

The crystal structure shows that Cu(II) is coordinated by four thiocyanate anions (μ-1,3) and two pyridine ligands adopting a slightly distorted octahedral coordination environment (CuS2N4). The Cu-N(pyridine) axial bonds are of length (Cu(1)-N(1) 2.045(3) Å, Cu(1)-N(2) 2.051(3) Å, Cu(2)-N(6)#1 1.943(3) Å, Cu(2)-N(5)#1 2.038(3) Å), while the equatorial Cu-N(thiocyanate) bonds (Cu(1)-N(3) 1.944(3) Å, Cu(1)-N(4) 1.951(3) Å). These bond lengths are similar to those found in the literature (Chen et al., 2005; Wohlert, Wriedt, Jess, & Nather, 2011). The Cu-S bonds (Cu1-S3 2.984(1) Å, Cu1-S1 2.994(1) Å, Cu1-S2 2.998(1) Å, Cu2-S2 3.069(1) Å) are also close to reported values (Chen et al., 2005). Adjacent Cu centres are bridged by two SCN− ions resulting in a 1D polymeric chain structure extending along the crystallographic c-axis (Figure 4). The Cu1-Cu1 and Cu2-Cu2 distances within the chains are 8.669 Å while that of Cu1-Cu2 is 5.616 Å. In the equatorial plane, the SCN− ion is almost linear as evidenced by the bond angles N(3)-C(11)-S(1) 179.0(3)° and N(4)-C(12)-S(2) 179.4(4)°. The pyridine molecules are...
almost linearly arranged on the axial plane as confirmed by the bond angle N(1)-Cu(1)-N(2) (178.06°). These results are similar to those reported in literature (Małecki, Machura, Świtlicka, Gron, & Balanda, 2011). The SCN⁻ and pyridine ligands are in different planes at right angles to each other as evidenced by the bond angles N(3)-Cu(1)-N(2) 89.66(12) and N(6)-Cu(2)-N(5) (90.36°). Selected crystal data of a polymorph of the complex are compared with crystal data of the title complex in Table 3. The title complex differs structurally from that in the literature (Chen et al., 2005) in terms of molecular weight, unit cell parameters and the number of atoms in a unit cell. The methods of syntheses of these complexes also differ.

Adjacent 1-D chains are further connected to form a 2-D supramolecular layer parallel to the bc plane by alternating S1…S3, S2…S2 (3.567(1) Å) and S3…S1 (3.541(1) Å) interactions as shown in Figure 5. This is similar to literature reports (Lu, Liu, Zhang, Wang, & Niu, 2010). The two-dimensional layers are further connected by off-set π–π stacking of pyridine rings, C–H…S and C–H…C interactions (Table 4) to form a three-dimensional supramolecular structure as shown in Figure 6 (Gerlach et al., 2015; Laachir, Bentiss, Guesmi, Saadi, & El Ammari, 2016; Trivedi, Pandey, & Rath, 2009). These

Table 3. Selected bond lengths (Å) and angles (°) for [Cu(Py)₂(SCN)₂]ₙ

| Bond/Angle | Value               |
|------------|---------------------|
| Cu(1)-N(3) | 1.944(3)            |
| Cu(1)-N(4) | 1.951(3)            |
| Cu(1)-N(1) | 2.045(3)            |
| Cu(1)-N(2) | 2.051(3)            |
| N(1)-C(5)  | 1.327(5)            |
| N(1)-C(1)  | 1.347(4)            |
| N(2)-C(10)| 1.337(5)            |
| N(2)-C(6)  | 1.344(4)            |
| N(3)-C(11)| 1.164(5)            |
| N(4)-C(12)| 1.164(5)            |
| Cu(2)-N(6)| 1.943(3)            |
| Cu(2)-N(6)#1| 1.943(3)         |
| Cu(2)-N(5) | 2.038(3)            |
| Cu(2)-N(5)#1| 2.038(3)          |
| N(5)-C(17)| 1.337(4)            |
| N(5)-C(13)| 1.346(4)            |
| N(6)-C(18)| 1.167(5)            |

Figure 5. Part of the crystal structure showing the formation, through S…S contacts, of the two-dimensional supramolecular sheet extending in the bc plane.
interactions, though weak compared to the metal–nitrogen and metal–sulphur coordination bonds, are crucial in the self-assembly of the 3D supramolecular structure.

### 3.3. IR spectroscopy

In the spectrum of the pyridine ligand as well as that of the complex, the absorption bands at 1,442 cm$^{-1}$ are assigned to the aryl C–H stretching vibrations. The $\nu_{\text{C}=\text{N}}$ stretching modes of the pyridine ring shifted from 1,595 to 1,604 cm$^{-1}$ in the spectrum of the complex, indicating its participation in bonding. The $\nu_{\text{C}=\text{N}}$ asymmetric stretching vibrations of the thiocyanate have shifted from 2,063 to 2,087 cm$^{-1}$ in the spectrum of the complex, indicating it has taken part in bonding (Kabesova & Gazo, 1980). The $\nu_{\text{SC}}$ vibration frequency of the isothiocyanato ligand appears at 746 cm$^{-1}$ on the SCN$^-$ spectrum and shifts to 753 cm$^{-1}$ on the spectrum of the complex, indicating NCS-M coordination in the complex (Kabesova & Gazo, 1980). These bands indicate the coordination of SCN$^-$ in a bridging mode (Shen & Feng, 2002), which is confirmed by the crystal structure of the complex. The strong, well-resolved and sharp absorption bands found in the region of 1,495–1,000 cm$^{-1}$ in the spectrum of the complex are assigned to the coordinated pyridine ring (Das et al., 2012). The $\nu_{\text{Cu-Npy}}$ stretching mode is present at about 549 cm$^{-1}$.

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**Table 4. Comparative crystal data of the complexes**

| Parameter              | $[\text{Cu}_3(\text{py})_6(\text{SCN})]_n$ [this work] | $[\text{Cu}(\text{py})_2(\text{SCN})]_n$ [33] |
|------------------------|------------------------------------------------------|-----------------------------------------------|
| Empirical formula      | $\text{C}_{36}\text{H}_{30}\text{Cu}_3\text{N}_{12}\text{S}_6$ | $\text{C}_{12}\text{H}_{10}\text{CuN}_4\text{S}_2$ |
| Formula weight         | 1,013.70                                             | 337.90                                        |
| Colour                 | Block blue                                           | Black blue                                    |
| Crystal system         | Triclinic                                            | Triclinic                                     |
| Space group            | $P \bar{1}$                                         | $P \bar{1}$                                   |
| Unit cell dimensions   |                                                      |                                               |
| $a$                    | 8.5381(6) Å                                         | 8.528(2) Å                                    |
| $b$                    | 8.6690(8) Å                                         | 9.128(1) Å                                    |
| $c$                    | 15.5456(9) Å                                        | 15.371(1) Å                                   |
| $\alpha$               | 93.367(6)$^\circ$                                   | 91.737(1)$^\circ$                             |
| $\beta$                | 96.385(5)$^\circ$                                   | 97.043(1)$^\circ$                             |
| $\gamma$               | 114.746(8)$^\circ$                                  | 115.639(1)$^\circ$                            |
| Unit cell volume, $V$  | 1,031.40(13) Å                                      | 1,065.9(3) Å                                  |
| Calc. density          | 1.632 mg m$^{-3}$                                    | 1.579 mg m$^{-3}$                             |
| $Z$                    | 1                                                    | 3                                             |
3.4. UV–Vis spectroscopy
The electronic absorption spectrum of the complex shows a single broad band centred at 15,625 cm\(^{-1}\) (640 nm). This d–d transition band in the Cu(II) ion has been assigned to \(2\text{E}_g \rightarrow 2\text{T}_{2g}\) transition (Kurdziel, Głowia̧k, Materazzi, & Jezierska, 2003; Rapheal, Manoj, & Kurup, 2007; Reddy, Nethaji, & Chakravarty, 2002). The observed band is consistent with an octahedral geometry for Cu(II) complexes as confirmed by the single X-ray crystal structure. This value is smaller than that of Cu(en)\(_2\)(SCN)\(_2\) (19,047 cm\(^{-1}\); 525 nm) and Cu(en)\(_2\)[Cd(SCN)\(_3\)]\(_2\) (18,248 cm\(^{-1}\); 548 nm) (Shen & Feng, 2002) with analogous CuN\(_4\)S\(_2\) chromophores. This shift in band position indicates some distortion from the perfect octahedral symmetry of Cu(II) (Bai et al., 2008).

3.5. Thermal analysis
In order to establish the thermal stability of the title complex, TG/DTA analyses were carried out in the temperature range of 30–600°C. The thermal decomposition thermogram (Figure 7) shows that the complex decomposes in several steps resulting in different phases of [Cu\(_3\)(Py)\(_6\)(SCN)\(_6\)]\(_n\) as temperature was increased. The first weight loss of 5.62% from 80 to 120°C is probably due to the loss of adsorbed water molecules from the atmosphere. The second degradation step in the range of 130–220°C with mass loss of 43.92% is attributed to the loss of six pyridine molecules (calculated 46.76%). The sharp exothermic DTA peak at 170°C indicates that this is the major decomposition temperature. The third degradation step in the range of 260–460°C with weight loss of 14.92% is due to the loss of three SCN\(^-\) anions (calculated 17.16%). In the last decomposition step from 510 to 590°C with mass loss of 8.48% is attributed to the loss of one SCN\(^-\) and CN\(^-\) (calculated 8.29%). A stable mass is reached at 600°C. The residual mass 27.96% (calculated 28.56%) is probably due to CuS. The measured mass loss for each stage is in good agreement with the calculated values.

3.6. Photoluminescence studies
The fluorescence emission spectra of the ligand and the complex are shown in Figure 8. The results show that the ligand pyridine and the complex exhibit only one emission peak each at 23,923 cm\(^{-1}\) (418 nm) and 24,509 cm\(^{-1}\) (408 nm), respectively, when excited at 33,333 cm\(^{-1}\) (300 nm). For the ligand, the peak at 23,923 cm\(^{-1}\) is attributed to n\(\rightarrow\)π* transition. The red shift of 10 nm in the spectrum of the complex indicates charge transfer from ligand to the metal (PyN\(\rightarrow\)Cu) (Etaiw & Abdou, 2016; Rapheal et al., 2007).
3.7. Antimicrobial studies

The effects of the starting materials, the resulting complex, the reference antibiotic (chloramphenicol) and antifungal (nystatin) were evaluated against some selected microbial pathogens (four bacteria and four fungi strains). The susceptibility of the bacteria and fungi strains towards these compounds was judged by measuring the size of the growth inhibition diameter. The diameter of the zone of inhibition (mm) was used to compare the antimicrobial activity of the test compound with that of the reference antibiotic and antifungal. Results of the preliminary screening are presented in Table 5.

The results indicate that SCN$^-$ exhibits a high activity against the pathogens, especially the fungi species. The metal complex shows higher activity compared to that of the free ligand as well as SCN. It was found to be active against all the pathogens with high inhibition zones. The complex is most active against the fungi C. albicans 194B, C. glabrata 44B and the bacteria species P. aeruginosa and S. typhi. The complex is also more active than the reference drug nystatin towards the fungi species. The most sensitive bacteria species was S. typhi. This indicates that reaction of metal ions with the ligand plays an important role in enhancing its antimicrobial activity. This increase in activity could be due to the reduction of the polarity of the metal ion by partial sharing of the positive charge with the ligand’s donor atoms so that there is electron delocalization within the metal complex. This may increase the hydrophobic and lipophilic character of the metal complex, enabling it to permeate the lipid layer of the organism killing them more effectively (Tabong et al., 2016; Yuoh et al., 2015).

4. Conclusion

A Cu(II) complex with SCN$^-$ and pyridine $[\text{Cu}_3(\text{py})_6(\text{SCN})_6]_n$ has been synthesized and characterized. The structure is polymorphic to $[\text{Cu}(\text{py})_2(\text{SCN})_2]_n$ (Chen et al., 2005) and iso-structural with $[\text{Ni}(\text{NCS})_2(\text{pyridine})_2]_n$ (Neumann et al., 2014). The crystal structure consists of two crystallographically independent copper(II) atoms, of which one (Cu1) is located on a general position whereas the second (Cu2) is located on a crystallographic inversion centre. Each Cu (II) atom adopts a slightly
distorted octahedral coordination environment (CuS₃N₄) in which it is covalently bonded to two pyridine N-atoms in the axial position, two S-atoms of SCN⁻ and two N-atoms of SCN⁻ in the equatorial position. Adjacent Cu centres are bridged by two SCN⁻ (μ-1,3) ions resulting in a 1D polymeric chain structure. Adjacent 1-D chains are further connected to form a 2-D supramolecular layer parallel to the bc plane by alternating S₁...S₃, S₂...S₂ (3.567(1) Å) and S₃...S₁ (3.541(1) Å), interactions. The two-dimensional layers are further connected by off-set π–π stacking of pyridine rings, C–H...S and C–H...C interactions to form a three-dimensional supramolecular structure. The complex exhibited photoluminescent properties in the solid state at room temperature because of charge transfer from ligand to the metal. The results of the preliminary antimicrobial screening against four pathogenic bacteria and four fungi species indicate that the complex is most active against S. typhi.

Supporting Information
CCDC 1055785 contains the supplementary crystallographic data for the complex. The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif. (or from the Cambridge Crystallographic Data Center, 12 Union Road, Cambridge CB21 1EZ, UK; Fax: +44 1223/363 033; E-mail: deposit@ccdc.cam.ac.uk).

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