Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[[(2-amino-5-bromopyridine-κN)copper(I)]-μ_3-iodo]

Aliakbar Dehno Khalaji,[a] Mehdi Amirnasr[a] and Jean-Claude Daran[b]*

[a]Department of Chemistry, Isfahan University of Technology, Isfahan 84156-83111, Iran, and [b]Laboratoire de Chimie de Coordination, CNRS UPR8241, 205 route de Narbonne, 31077 Toulouse Cedex, France

Correspondence e-mail: daran@lcc-toulouse.fr

Received 27 October 2006
Accepted 31 October 2006

In the crystal structure of the title compound, $[CuI(C_5H_5BrN_2)]_n$, the Cu and I atoms form Cu–I polymeric double chains in which each Cu atom is coordinated by three I atoms and one N atom of a 2-amino-5-bromopyridine ligand in a distorted tetrahedral geometry. The chains are linked by N—H···N hydrogen bonds, forming layers parallel to the (001) plane.

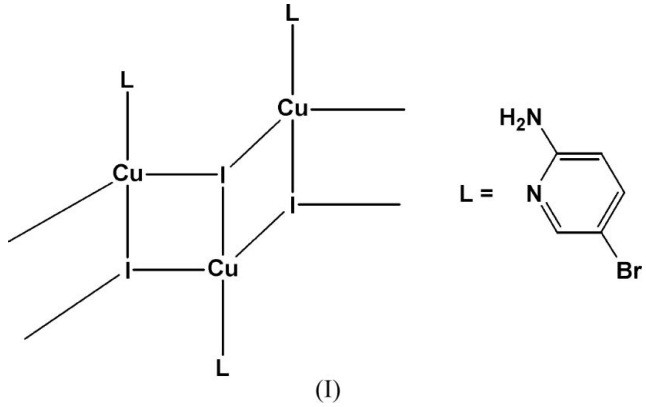
Key indicators

Single-crystal X-ray study
T = 180 K
Mean σ(C–C) = 0.004 Å
R factor = 0.022
wR factor = 0.052
Data-to-parameter ratio = 21.7

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

Inorganic copper(I) coordination polymers based on copper(I) halides or pseudohalides and aromatic nitrogen-donor ligands are well known and several of them have been synthesized and characterized in the past. These compounds consist of copper halide substructures, such as four- or six-membered rings, which are connected by the *N*-donor ligands to give one-, two- or three-dimensional coordination polymers (Graham *et al.*, 2000; Näther & Jess, 2002; Goher & Mautner, 1999; Persky *et al.*, 2001; Näther *et al.*, 2001, 2003). When copper(I) halides are combined with monodentate ligands, the occurrence of bridging halides produces a wide variety of oligomeric structures, such as monomeric (Davis *et al.*, 1973), square dimeric (Churchill & Rotella, 1979), cubane tetrameric (Pike *et al.*, 1999), zigzag polymeric (Healy *et al.*, 1989*a*) and stair-step oligomeric structures (Healy *et al.*, 1989*b*). Here we report the synthesis and crystal structure of the roof-shaped copper(I) polymer poly[[(2-amino-5-bromopyridine-κN)-copper(I)]-μ_3-iodo], (I).



(I)

Each Cu^I atom is coordinated by three I atoms and one N atom of a 2-amino-5-bromopyridine ligand in a distorted tetrahedral geometry (Fig. 1). The bond lengths and angles are similar to those of related compounds (Graham *et al.*, 2000; Näther & Jess, 2002; Goher *et al.*, 1999; Persky *et al.*, 2001). The Cu atoms are connected through the I atoms, forming a roof-

shaped copper(I) polymer (Fig. 1). The polymeric chains are connected through N—H···N hydrogen bonds (Table 1), leading to the formation of layers parallel to the (001) plane (Fig. 2).

Experimental

To a stirred solution of CuI (945 mg, 0.5 mmol) in acetonitrile (3 ml), a solution of 2-amino-5-bromopyridine (85 mg, 0.5 mmol) in acetonitrile (3 ml) was added dropwise at room temperature, and the mixture was stirred for 5 min. The volume of the solution was then reduced under vacuum to about 3 ml. Colourless crystals of (I) suitable for X-ray crystallographic analysis were obtained by the diffusion of diethyl ether vapour into the solution at 298 K. The crystals were collected by filtration and dried under vacuum.

Crystal data

$[CuI(C_5H_5BrN_2)]$
M_r = 363.46
Monoclinic, $P2_1/c$
a = 8.7391 (5) Å
b = 4.2118 (3) Å
c = 21.8958 (13) Å
β = 99.135 (5)°
V = 795.70 (9) Å^3
Z = 4
D_x = 3.034 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 11.57 mm^{-1}
T = 180 (2) K
Block, colourless
0.41 × 0.28 × 0.19 mm

Data collection

Oxford Diffraction XCALIBUR diffractometer
ω and φ scans
Absorption correction: analytical (Katayama, 1986)
T_{min} = 0.057, T_{max} = 0.154
6460 measured reflections
1979 independent reflections
1819 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
θ_{max} = 28.3°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.052
S = 1.17
1979 reflections
91 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0252P)^2 + 1.2505P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.74 e Å^{-3}
$\Delta\rho_{min}$ = −1.00 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H21···N2^{i}	0.91	2.40	3.191 (4)	145

Symmetry code: (i) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$.

H atoms attached to C atoms were placed in geometrically idealized positions and treated as riding on their parent atoms, with C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C). H atoms attached to the N atom were located in a difference Fourier synthesis but they were treated as riding on their parent atom, with N—H = 0.91 Å and U_{iso}(H) = 1.2U_{eq}(N).

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

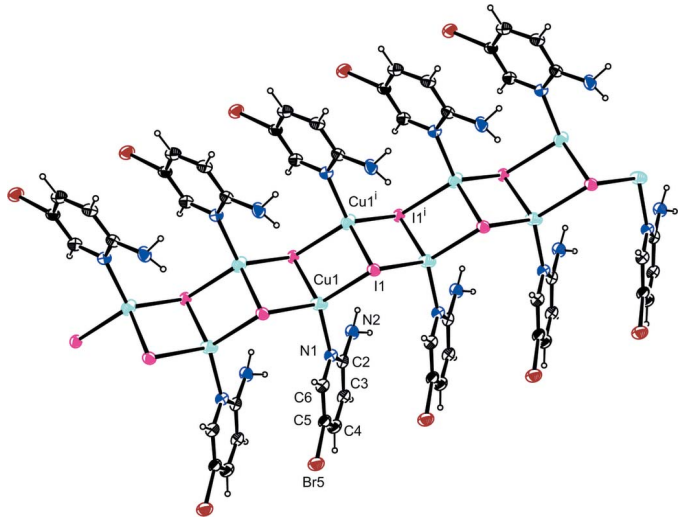


Figure 1
Part of the polymeric chain structure of (I), showing the coordination of the Cu^{I} atoms and the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level [symmetry codes: (i) $x, y-1, z$; (ii) $x, 1-y, z$: (iii) $2-x, y-\frac{1}{2}, \frac{1}{2}-z$; (iv) $2-x, \frac{1}{2}+y, \frac{1}{2}-z$].

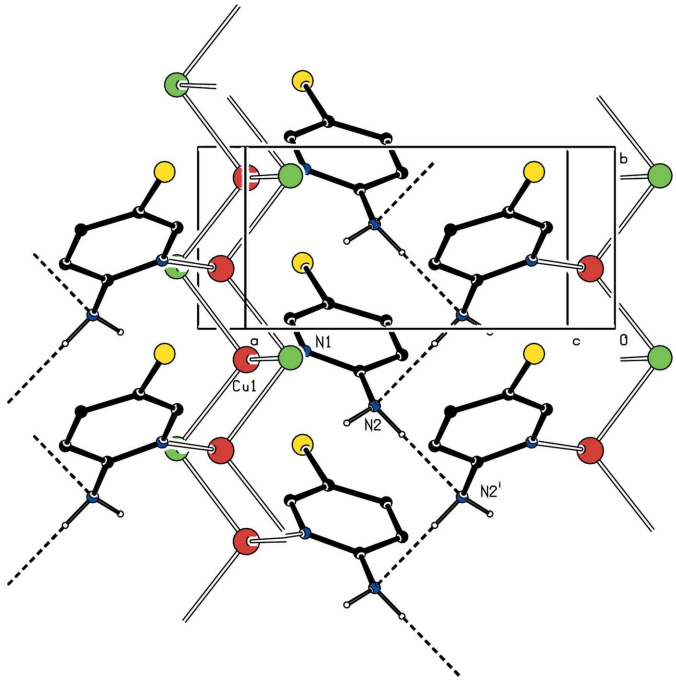


Figure 2
Partial packing view showing the N—H···N hydrogen-bonding interactions between the roof-shaped polymer chains (dashed lines). H atoms not involved in hydrogen-bonding interactions have been omitted for clarity [symmetry code: (i) $1-x, y-\frac{1}{2}, \frac{1}{2}-z$].

References

Altomare, A., Burla, M. C., Camalli, M., Cascarano, G. L., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.
Churchill, M. R. & Rotella, R. J. (1979). *Inorg. Chem.* **18**, 166–171.
Davis, P. H., Belford, R. L. & Paul, I. C. (1973). *Inorg. Chem.* **12**, 213–218.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.

Goher, M. A. S. & Mautner, F. A. (1999). *Polyhedron*, **18**, 1805–1810.
Graham, P. M., Pike, R. D., Sabat, M., Bailey, R. D. & Pennington, W. T. (2000). *Inorg. Chem.* **39**, 5121–5132.
Healy, P. C., Kildea, J. D., Skelton, B. W. & White, A. H. (1989*a*). *Aust. J. Chem.* **42**, 115–136.
Healy, P. C., Kildea, J. D., Skelton, B. W. & White, A. H. (1989*b*). *Aust. J. Chem.* **42**, 79–91.
Katayama, C. (1986). *Acta Cryst.* A**42**, 19–23.
Näther, C., Greve, J., Jess, I. & Wickleder, C. (2003). *Solid State Sci.* **5**, 1167–1176.
Näther, C. & Jess, I. (2002). *Z. Naturforsch. Teil B*, **57**, 1133–1140.
Näther, C., Jess, I. & Greve, J. (2001). *Polyhedron*, **20**, 1017–1022.
Oxford Diffraction (2006). *CrysAlis CCD* and *CrysAlis RED*. Versions 1.171.31.5. Oxford Diffraction Ltd., Abingdon, Oxfordshire, England.
Persky, N. S., Chow, J. M., Poschmann, K. A., Lacuesta, N. N., Stoll, S. L., Bott, S. G. & Obrey, S. (2001). *Inorg. Chem.* **40**, 29–35.
Pike, R. D., Starnes, W. H. & Carpenter, G. B. (1999). *Acta Cryst.* C**55**, 162–165.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.