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Key indicators

Single-crystal X-ray study
T = 220 K
Mean $\sigma(\text{C}-\text{C}) = 0.012 \text{ \AA}$
R factor = 0.052
wR factor = 0.140
Data-to-parameter ratio = 12.2

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

catena-Poly[[bis(2,2'-bipyridine- κ^2N,N')copper(II)]- μ -cyano-dicyanoplatinate(II)- μ -cyano]

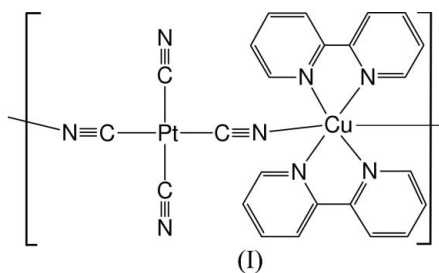
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The crystal structure of the title complex, $[\text{Cu}(\text{C}_{10}\text{H}_8\text{N}_2)_2[\text{Pt}(\text{CN})_4]]_n$, is built up by infinite neutral chains in which $[\text{Cu}(\text{bpy})_2]^{2+}$ (bpy = 2,2'-bipyridine) complex cations are bridged by $[\text{Pt}(\text{CN})_4]^{2-}$ complex anions. Two bridging cyano groups of $[\text{Pt}(\text{CN})_4]^{2-}$ anions are in *trans* positions with Pt—C distances of 2.000 (9) Å. Nevertheless, the chains are not linear but zigzag, owing to the *cis* coordination of the cyano groups to the Cu atom [Cu—N = 2.243 (8) Å]. The remaining four coordination sites of the Cu atom are occupied by N atoms of two chelating bpy molecules at distances of 2.022 (4) and 2.161 (6) Å. Cu atoms lie on twofold rotation axes and Pt atoms on inversion centres.

Comment

Because tetracyanoplatinate(II) anions can use a different number of cyano groups to bind to other metal atoms, they exist in a wide range of solid-state structures (Pilkington *et al.*, 2004). The complete scheme of bonding modes of $[\text{Pt}(\text{CN})_4]^{2-}$ anions is given in our previous paper dealing with magnetostructural correlation of the $[\text{Cu}(\text{en})_2][\text{Pt}(\text{CN})_4]$ complex (en = ethylenediamine; Potočník *et al.*, 2006), the structure of which was published independently very recently (Akitsu *et al.*, 2006). The study of this compound, as well as of other $[\text{Cu}(\text{en})_2][M(\text{CN})_4]$ ($M = \text{Ni}, \text{Pd}$) compounds (Orendáč *et al.*, 1995; Černák *et al.*, 2001), revealed that, despite their one-dimensional structure, they behave as two-dimensional magnets. This two-dimensional character of the magnetic subsystem can be explained by the formation of relatively strong N—H...N hydrogen bonds (HBs) linking neighbouring chains. To eliminate these HBs we decided to replace en by other ligands which cannot be involved in HB systems, such as methyl derivatives of en or aromatic ligands such as 1,10-phenanthroline or 2,2'-bipyridine. In this paper, we present the crystal structure of $[\text{Cu}(\text{bpy})_2][\text{Pt}(\text{CN})_4]$, (I).



The crystal structure of (I) consists of infinite chains; part of one chain is shown in Fig. 1. These chains are formed by $[\text{Cu}(\text{bpy})_2]^{2+}$ complex cations, with Cu^{II} atoms placed on

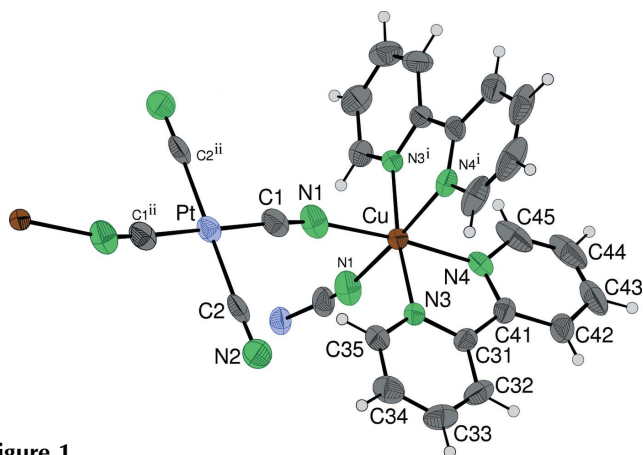


Figure 1
A segment of the polymeric structure of (I) with the atom-labelling scheme. Displacement ellipsoids are drawn at the 40% probability level and H atoms are shown as small spheres of arbitrary radii. [Symmetry codes: (i) $-x, y, -z + \frac{1}{2}$; (ii) $-x, -y, -z$.]

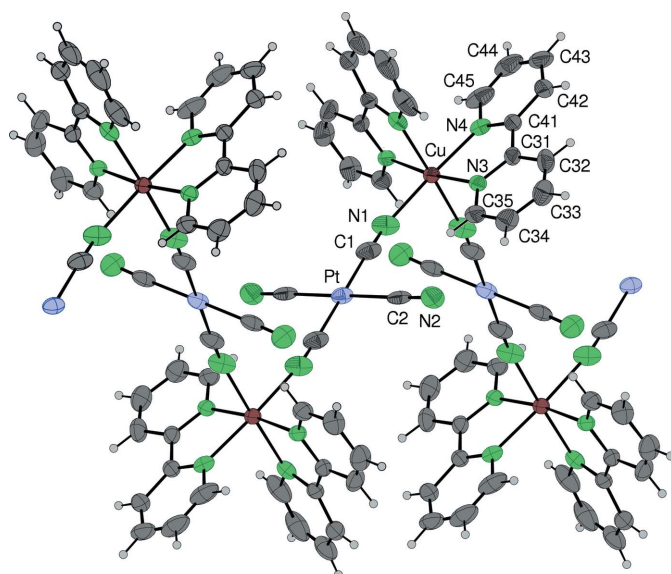


Figure 2
Zigzag chain in (I). Displacement ellipsoids are drawn at the 40% probability level and H atoms are shown as small spheres of arbitrary radii.

twofold rotation axes, connected by $[\text{Pt}(\text{CN})_4]^{2-}$ complex anions with Pt^{II} atoms lying on inversion centres. Two bridging cyano groups of the square-planar tetracyanoplatinate anion are coordinated in *trans* positions with $\text{Pt}-\text{C}$ distances of 2.000 (9) Å, while the terminal cyano groups are at distances of 1.997 (10) Å. Despite the *trans* coordination of the bridging cyano groups in the $[\text{Pt}(\text{CN})_4]^{2-}$ anion, the chains are not linear but zigzag (Fig. 2). This is caused by *cis* coordination of the bridging cyano groups to the Cu atoms at 2.243 (8) Å, with an $\text{N1}-\text{Cu}-\text{N1}^i$ angle of 89.3 (4)° [symmetry code: (i) $-x, y, \frac{1}{2} - z$]. The four remaining N atoms of the slightly deformed octahedron are coordinated at somewhat shorter distances of 2.022 (4) and 2.161 (6) Å and originate from two chelating bpy molecules. The structure may be stabilized by very a weak HB system established by $\text{C35}-\text{H35}\cdots\text{N1}$ bonds within one chain

(Table 2). Nevertheless, these HBs cannot be compared with the relatively strong HBs connecting neighbouring chains in $[\text{Cu}(\text{en})_2][\text{M}(\text{CN})_4]$ ($M = \text{Ni}, \text{Pd}$ or Pt) compounds.

Experimental

Crystals of (I) were prepared by mixing a 20 ml water–methanol (1:1) solution of CuSO_4 (0.5 mmol) with a 20 ml water–methanol (1:1) solution of bpy (2 mmol) and, after 30 min of stirring, 10 ml of an aqueous solution of $\text{K}_2[\text{Pt}(\text{CN})_4]$ (0.5 mmol) was added. The blue precipitate thus formed was dissolved by addition of a concentrated solution of ammonia (15 ml). After one week, blue crystals of (I) were filtered off and dried in air.

Crystal data

$[\text{CuPt}(\text{C}_{10}\text{H}_8\text{N}_2)_2(\text{CN})_4]$	$Z = 4$
$M_r = 675.08$	$D_x = 1.983 \text{ Mg m}^{-3}$
Orthorhombic, <i>Pbcn</i>	Mo $K\alpha$ radiation
$a = 13.167 (2) \text{ \AA}$	$\mu = 7.15 \text{ mm}^{-1}$
$b = 11.055 (2) \text{ \AA}$	$T = 220 (1) \text{ K}$
$c = 15.534 (2) \text{ \AA}$	Plate, blue
$V = 2261.2 (7) \text{ \AA}^3$	$0.60 \times 0.57 \times 0.11 \text{ mm}$

Data collection

Stoe IPDS diffractometer	11207 measured reflections
φ scans	1923 independent reflections
Absorption correction: numerical (<i>FACE</i> in <i>IPDS Software</i> ; Stoe & Cie, 1999)	1377 reflections with $I > 2\sigma(I)$
$T_{\text{min}} = 0.049, T_{\text{max}} = 0.444$	$R_{\text{int}} = 0.103$
	$\theta_{\text{max}} = 25.1^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0926P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.052$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.140$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.00$	$\Delta\rho_{\text{max}} = 1.16 \text{ e \AA}^{-3}$
1923 reflections	$\Delta\rho_{\text{min}} = -2.65 \text{ e \AA}^{-3}$
157 parameters	Extinction correction: <i>SHELXL97</i>
H-atom parameters constrained	Extinction coefficient: 0.0077 (7)

Table 1

Selected geometric parameters (Å, °).

$\text{Pt}-\text{C2}$	1.997 (10)	$\text{Cu}-\text{N1}$	2.243 (8)
$\text{Pt}-\text{C1}$	2.000 (9)	$\text{N1}-\text{C1}$	1.150 (11)
$\text{Cu}-\text{N3}$	2.022 (4)	$\text{N2}-\text{C2}$	1.145 (11)
$\text{Cu}-\text{N4}$	2.161 (6)		
$\text{C2}-\text{Pt}-\text{C1}$	88.2 (3)	$\text{N4}-\text{Cu}-\text{N1}$	172.7 (2)
$\text{N3}-\text{Cu}-\text{N3}^i$	172.5 (3)	$\text{N4}^i-\text{Cu}-\text{N1}$	92.4 (2)
$\text{N3}-\text{Cu}-\text{N4}$	78.4 (2)	$\text{N1}-\text{Cu}-\text{N1}^i$	89.3 (4)
$\text{N3}^i-\text{Cu}-\text{N4}$	96.1 (2)	$\text{C1}-\text{N1}-\text{Cu}$	164.8 (6)
$\text{N4}-\text{Cu}-\text{N4}^i$	86.8 (3)	$\text{N2}-\text{C2}-\text{Pt}$	177.2 (8)
$\text{N3}-\text{Cu}-\text{N1}$	94.5 (2)	$\text{N1}-\text{C1}-\text{Pt}$	176.9 (6)
$\text{N3}^i-\text{Cu}-\text{N1}$	90.9 (2)		

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C35}-\text{H35}\cdots\text{N1}$	0.93	2.51	3.136 (9)	125

All H atoms positions were calculated using a riding model (C–H = 0.93 Å) with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The highest residual density peak is located 2.51 Å from atom N4 and the deepest hole is 1.00 Å from the Pt atom.

Data collection: *EXPOSE* in *IPDS Software* (Stoe & Cie, 1999); cell refinement: *CELL* in *IPDS Software*; data reduction: *INTEGRATE* in *IPDS Software*; program(s) used to solve structure: *SHELXS86* (Sheldrick, 1985); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2000); software used to prepare material for publication: *SHELXL97*.

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