Acta Crystallographica Section E
**Structure Reports**
**Online**
ISSN 1600-5368

# Bis(2,2′-bipyridine-$\kappa^2N,N'$)(nitrato-$\kappa O$)copper(II) hexafluorophosphate

**Garikoitz Beobide, Oscar Castillo,* Urko García-Couceiro, Juan P. García-Terán and Antonio Luque**

Departamento de Química Inorgánica, Facultad de Ciencia y Tecnología, Universidad del País Vasco, Apdo. 644, E-48080 Bilbao, Spain

Correspondence e-mail: oscar.castillo@ehu.es

The title compound, $[Cu(NO_3)(C_{10}H_8N_2)_2]PF_6$, comprises $[Cu(NO_3)(bpy)_2]^+$ complex cations (bpy = 2,2′-bipyridine) and uncoordinated $PF_6^-$ anions. The $Cu^{II}$ ion is five-coordinated in a distorted trigonal bipyramidal fashion by two bpy molecules and one nitrate anion, which is coordinated in an equatorial position through one O atom at a distance of 2.148 (3)Å. The two axial Cu—N distances are similar (mean = 1.98Å) and are slightly shorter than the two equatorial Cu—N bonds (mean = 2.06Å). Longer Cu···O interactions exist between complexes, linking them into polymeric chains.

Received 24 April 2006
Accepted 16 May 2006

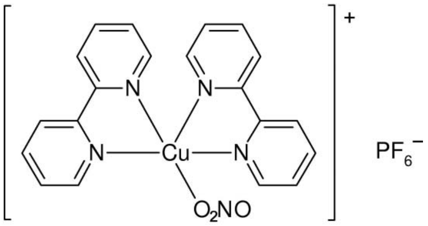
**Key indicators**

Single-crystal X-ray study
$T$ = 293 K
Mean $\sigma$(C–C) = 0.006 Å
$R$ factor = 0.040
$wR$ factor = 0.071
Data-to-parameter ratio = 12.0

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

## Comment

Copper–bipyridine complexes have been proposed as catalysts for the hydrolysis of phosphate triesters, such as those found in toxic nerve agents (Morrow & Trogler, 1989). We report here the crystal structure of a new copper bipyridine (bpy) complex, namely bis(2,2′-bipyridine)nitratocopper(II) hexafluorophosphate, (I). The structure comprises $[Cu(NO_3)(bpy)_2]^+$ cations (Fig. 1) and $PF_6^-$ anions. The $Cu^{II}$ ion is located on a general position and is coordinated in a trigonal–bipyramidal geometry by two bipyridine ligands and one nitrate anion (Table 1).



(I)

The pyridine rings in both the N11–C112 and N21–C212 bpy ligands are twisted with respect to each other around the central C—C bond, forming dihedral angles between the ring planes of 9.7 (1) and 2.1 (1)°, respectively. The axial Cu—N11 and Cu—N21 distances are nearly equal and almost collinear (Table 1). The angles among the axial and equatorial donor atoms lie within the range 80.03 (13)–102.77 (13)°. The equatorial N18—Cu1—N28 bond angle is close to an ideal angle of 120°, while the two remaining bond angles differ considerably from the ideal trigonal angle, with one large (N28—Cu1—O1) and one small angle (N18—Cu1—O1). The Addison parameter (Addison *et al.*, 1984), $\tau$ = 0.603, is indicative of a distorted trigonal bipyramid.

Longer Cu···O interactions are formed between complexes [O3···Cu1$^i$ = 3.457 (3) Å; symmetry code: (i) −1 + $x$, $y$, $z$], linking them into polymeric chains along the $a$ axis (Fig. 2).

doi:10.1107/S1600536806018083

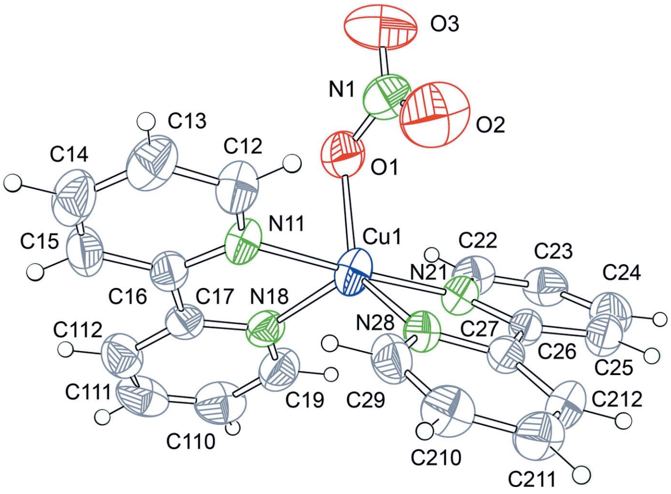


**Figure 1**
A view of the cationic complex in (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are drawn as spheres of arbitrary radii.

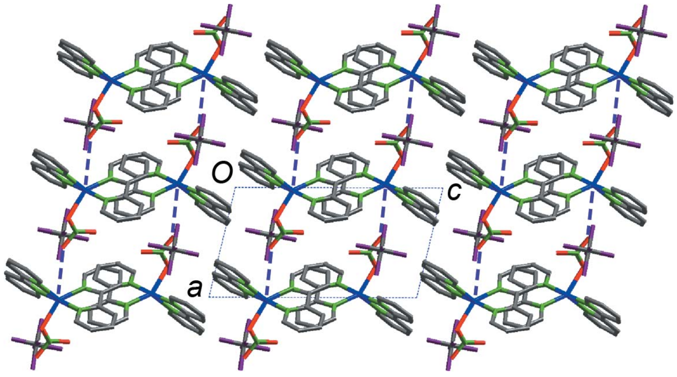


**Figure 2**
The packing, viewed along the *b* axis. Thick dashed lines denote Cu$\cdots$O interactions linking the complexes into polymeric chains. H atoms have been omitted.

Aromatic stacking interactions are established between the pyridine rings of the N21–C212 bpy ligands in adjacent chains (Fig. 3). Two different interactions are formed: centroid(N21–C26)$\cdots$centroid(N21–C26)$^{ii}$ = 3.56 Å; centroid(C27–C212)$\cdots$centroid(N28–C212)$^{iii}$ = 3.65Å [symmetry codes: (ii) $-x$, $-y$, $1 - z$; (iii) $-x$, $1 - y$, $1 - z$]. Further stacking interactions exist between N11–C112 bpy ligands: centroid(N11–C16)$\cdots$centroid(C17–C112)$^{iv}$ = 3.75 Å [symmetry code: (iv) $-x$, $1 - y$, $2 - z$]. The $PF_6^-$ counter-ions are situated in the holes generated by the packing of the cationic complexes.

## Experimental

Crystals of (I) were prepared by mixing a methanolic solution (10 ml) of 2,2′-bipyridine (0.0937 g, 0.6 mmol) and an aqueous solution (15 ml) of $Cu(NO_3)_2\cdot H_2O$ (0.1450 g, 0.6 mmol). To the resulting blue solution, an aqueous solution (5 ml) of $KPF_6$ (0.0552 g, 0.3 mmol) was added. After a few days, blue crystals of the title compound were filtered off and dried in air.

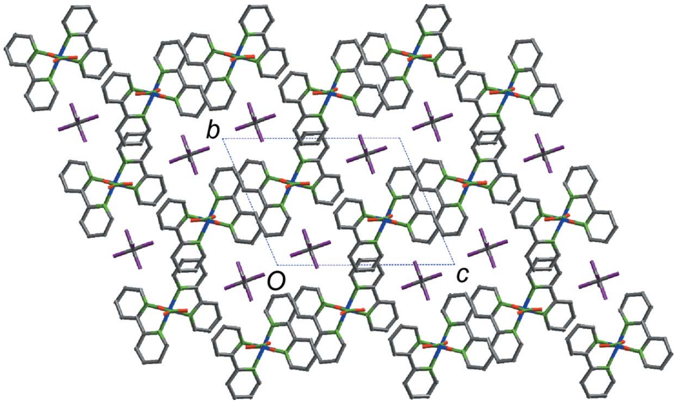


**Figure 3**
The packing, viewed along the *a* axis, showing $PF_6^-$ anions lying between the cationic complexes. H atoms have been omitted.

*Crystal data*

$[Cu(NO_3)(C_{10}H_8N_2)_2]PF_6$
$M_r = 582.89$
Triclinic, $P\bar{1}$
$a = 7.449$ (1) Å
$b = 11.329$ (2) Å
$c = 14.564$ (2) Å
$\alpha = 111.27$ (2)°
$\beta = 99.16$ (1)°
$\gamma = 98.52$ (2)°
$V = 1102.0$ (3) Å$^3$
$Z = 2$
$D_x = 1.756$ Mg m$^{-3}$
$D_m = 1.75(1)$ Mg m$^{-3}$
$D_m$ measured by flotation in a mixture of carbon tetrachloride and bromoform
Mo $K\alpha$ radiation
$\mu = 1.15$ mm$^{-1}$
$T = 293$ (2) K
Prism, blue
0.30 × 0.20 × 0.20 mm

*Data collection*

Oxford Diffraction Xcalibur CCD diffractometer
$\omega$ scans
Absorption correction: none
7697 measured reflections
3894 independent reflections
1939 reflections with $I > 2\sigma(I)$
$R_{int} = 0.040$
$\theta_{max} = 25.0°$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.071$
$S = 0.74$
3894 reflections
325 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0217P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.34$ e Å$^{-3}$
$\Delta\rho_{min} = -0.32$ e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Cu1—N11 | 1.979 (3) | Cu1—N28 | 2.025 (3) |
| Cu1—N18 | 2.092 (3) | Cu1—O1 | 2.148 (3) |
| Cu1—N21 | 1.980 (3) | | |
| N11—Cu1—N18 | 80.03 (13) | N21—Cu1—N28 | 80.99 (12) |
| N21—Cu1—N18 | 102.77 (13) | N11—Cu1—O1 | 88.16 (11) |
| N28—Cu1—N18 | 126.41 (11) | N18—Cu1—O1 | 92.77 (11) |
| N11—Cu1—N21 | 176.97 (13) | N21—Cu1—O1 | 90.55 (12) |
| N11—Cu1—N28 | 98.32 (12) | N28—Cu1—O1 | 140.81 (11) |

H atoms were included at calculated positions and treated as riding atoms [C—H = 0.93Å and $U_{iso}(H) = 1.2U_{eq}(C)$]. The relatively large displacement parameters for atoms O2 and O3 suggest minor disorder for the nitrate anion; this was not modelled.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2003); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford

Diffraction, 2003); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

This work was supported by the Ministerio de Educacón y Ciencia (MAT2005–03047) and the Universidad del País Vasco/Euskal Herriko Unibertsitatea (9/UPV 00169.310–15329/2003). GB thanks Eusko Jaurlaritza/Gobierno Vasco for a predoctoral fellowship.

## References

Addison, A. W., Rao, T. N., Reedijk, J., van Rijn, J. & Verschoor, G. C. (1984). *J. Chem. Soc. Dalton Trans.* pp. 1349–1356.
Altomare, A., Cascarano, G., Giacovazzo, C. & Guagliardi, A. (1993). *J. Appl. Cryst.* **26**, 343–350.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Morrow, J. R. & Trogler, W. C. (1989). *Inorg. Chem.* **28**, 1330–2333.
Oxford Diffraction (2003). *CrysAlis CCD* and *CrysAlis RED*. Versions 1.170. Oxford Diffraction, Wroclaw, Poland.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.