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Bis[3-(pyrazin-2-yl)-5-(pyridin-2-yl-κN)-1,2,4-triazol-1-ido-κN^1]copper(II)

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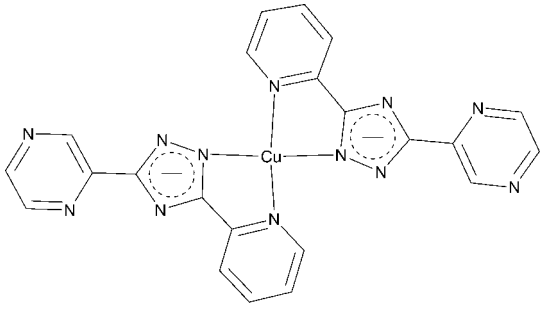
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.033; wR factor = 0.083; data-to-parameter ratio = 10.9.

In the mononuclear title complex, $[Cu(C_{11}H_7N_6)_2]$, the Cu^{II} atom lies on a crystallographic inversion centre and is coordinated by four N atoms from two bidentate chelate monoanionic 3-(pyrazin-2-yl)-5-(pyridin-2-yl-1,2,4-triazol-1-ido ligands, two from the triazolide rings [Cu—N = 1.969 (2) Å] and two from the pyridine rings [Cu—N = 2.027 (2) Å], giving a slightly distorted square-planar geometry.

Related literature

For details of the synthesis and properties of related copper compounds showing a similar coordination environment, see: Meng *et al.* (2009); Cheng *et al.* (2007); Zhang *et al.* (2005). For the structure of an Ru^{II} complex with the same ligand, see: Browne *et al.* (2002).



Experimental

Crystal data

$[Cu(C_{11}H_7N_6)_2]$
M_r = 509.99
Monoclinic, $P2_1/c$
a = 11.9735 (4) Å
b = 10.7539 (3) Å
c = 8.0162 (3) Å
β = 106.500 (4)°
V = 989.67 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.15 mm^{-1}
T = 293 K
0.20 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.795, T_{max} = 0.795
3248 measured reflections
1739 independent reflections
1451 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.083
S = 1.06
1739 reflections
160 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZS2193).

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supporting information

Acta Cryst. (2012). E**68**, m669 [doi:10.1107/S1600536812016777]

Bis[3-(pyrazin-2-yl)-5-(pyridin-2-yl-κN)-1,2,4-triazol-1-ido-κN^1]copper(II)

Lin-Lin Cong, Min-Yan Kang, Yu-Fei Ji and Zhi-Liang Liu

S1. Comment

2-(5-Pyridin-2-yl)-1,2,4-triazol-3-yl)pyrazine (Hptp) is a potentially multidentate ligand containing multiple *N* coordination sites. The synthesis and properties of copper complexes with similar ligands have been described (Meng *et al.*, 2009; Cheng *et al.*, 2007; Zhang *et al.*, 2005). However, only one crystal structure of a metal complex with the named ligand has been reported in the crystallographic literature, that with Ru (Browne *et al.*, 2002). Herein, we report the synthesis and crystal structure of the copper(II) complex with the ptp$^-$ ligand, the title complex $[Cu(C_{11}H_7N_6)_2]$.

As shown in Fig. 1, this complex is a discrete neutral monomer, in which the Cu^{II} atom resides on a crystallographic inversion centre. The Cu^{II} atom is in a slightly distorted $[N_4]$ square planar environment, with the coordination sphere defined by two pyridyl N-atom donors [Cu—$N_{pyridine}$ = 2.027 (2) Å] and two triazolate N-atom donors [Cu—$N_{triazolide}$ = 1.969 (2) Å] from two bidentate chelate ptp$^-$ anion ligands. The dihedral angle between the coordinated pyridyl group and the triazolato ring is 1.33 (9)°. In the crystal packing there are only minor weak intermolecular C—H···N hydrogen-bonding interactions (Table 1).

S2. Experimental

$CuCl_2 \cdot 2H_2O$ (1 mmol, 0.1704 g), Hptp (1 mmol, 0.2242 g), aqueous ammonia (25%, 2.0 ml) and water (15 ml) were heated in a 23-ml Teflon-lined autoclave at 160 °C for 3 days, followed by slow cooling (5 °C h^{-1}) to room temperature. The black block crystals were filtered off and washed with water (yield 42%, based on $CuCl_2 \cdot 2H_2O$). IR (KBr, cm^{-1}): 3424 (br), 3048 (w), 1620 (*s*), 1465 (*s*), 1401 (*m*), 1377 (*m*), 1120 (w), 1026 (w), 763 (*m*).

S3. Refinement

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H = 0.93 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$.

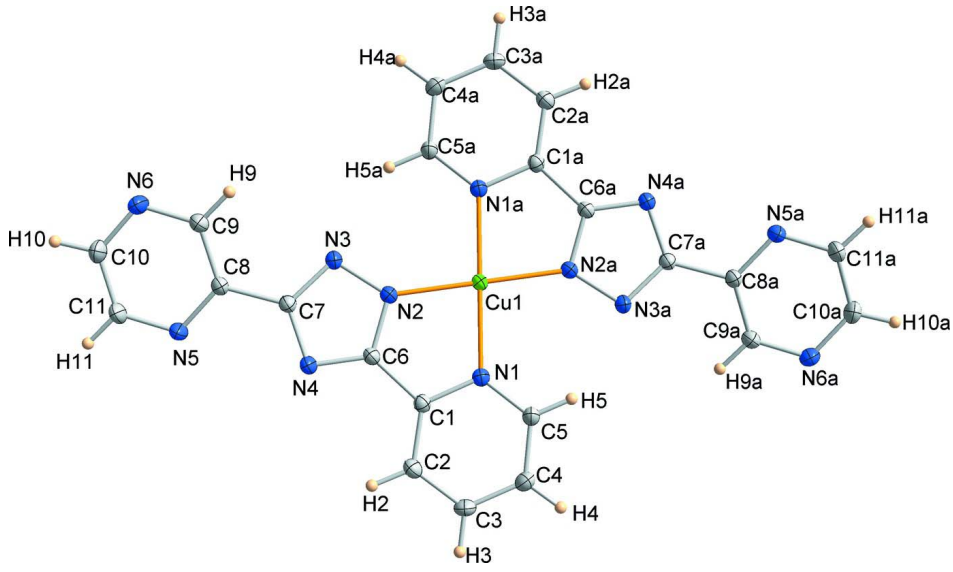

Figure 1

The molecular structure of the title complex, showing 30% probability displacement ellipsoids. For symmetry code (a): -*x* + 2, -*y* + 2, -*z*.

Bis[3-(pyrazin-2-yl)-5-(pyridin-2-yl-*κN*)-1,2,4-triazol-1-ido- *κN*^{1}]copper(II)

Crystal data

$[Cu(C_{11}H_7N_6)_2]$
M_r = 509.99
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 11.9735 (4) Å
b = 10.7539 (3) Å
c = 8.0162 (3) Å
β = 106.500 (4)°
V = 989.67 (6) Å^3
Z = 2
$F(000)$ = 518
D_x = 1.711 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2919 reflections
θ = 2.6–25.0°
μ = 1.15 mm^{-1}
T = 293 K
Block, black
0.20 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEX I diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.192 pixels mm^{-1}
ω–2θ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.795, T_{max} = 0.795
3248 measured reflections
1739 independent reflections
1451 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 25.0°, θ_{min} = 2.6°
h = −14→13
k = −11→12
l = −9→6

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.083
S = 1.06
1739 reflections
160 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0356P)^2 + 0.5521P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.28$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	1.00000	1.00000	0.00000	0.0286 (2)
N1	1.10513 (18)	0.85051 (18)	0.0123 (3)	0.0267 (7)
N2	0.91236 (19)	0.87911 (18)	0.0980 (3)	0.0288 (7)
N3	0.81241 (19)	0.87336 (18)	0.1478 (3)	0.0298 (7)
N4	0.88670 (18)	0.67872 (18)	0.1531 (3)	0.0282 (7)
N5	0.6786 (2)	0.5834 (2)	0.2120 (3)	0.0376 (8)
N6	0.5319 (2)	0.7455 (2)	0.3250 (3)	0.0398 (8)
C1	1.0605 (2)	0.7434 (2)	0.0551 (3)	0.0250 (8)
C2	1.1125 (2)	0.6297 (2)	0.0511 (3)	0.0319 (8)
C3	1.2139 (2)	0.6250 (2)	0.0029 (4)	0.0344 (9)
C4	1.2622 (2)	0.7337 (2)	−0.0353 (4)	0.0355 (9)
C5	1.2058 (2)	0.8444 (2)	−0.0294 (3)	0.0307 (8)
C6	0.9528 (2)	0.7623 (2)	0.1032 (3)	0.0257 (8)
C7	0.8009 (2)	0.7528 (2)	0.1784 (3)	0.0262 (8)
C8	0.6998 (2)	0.7053 (2)	0.2278 (3)	0.0258 (8)
C9	0.6261 (2)	0.7845 (2)	0.2850 (4)	0.0328 (9)
C10	0.5123 (3)	0.6236 (3)	0.3091 (4)	0.0420 (10)
C11	0.5841 (3)	0.5442 (3)	0.2539 (4)	0.0446 (10)
H2	1.07980	0.55750	0.08060	0.0380*
H3	1.24950	0.54900	−0.00390	0.0410*
H4	1.33200	0.73230	−0.06470	0.0430*
H5	1.23870	0.91770	−0.05530	0.0370*
H9	0.64390	0.86880	0.29570	0.0390*
H10	0.44770	0.59120	0.33650	0.0500*
H11	0.56640	0.45980	0.24520	0.0530*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0274 (3)	0.0210 (2)	0.0417 (3)	0.0025 (2)	0.0166 (2)	0.0069 (2)
N1	0.0255 (11)	0.0248 (11)	0.0306 (12)	−0.0007 (9)	0.0092 (9)	0.0017 (9)

N2	0.0296 (12)	0.0218 (11)	0.0384 (13)	0.0016 (9)	0.0150 (10)	0.0034 (9)
N3	0.0308 (12)	0.0241 (11)	0.0392 (13)	−0.0009 (10)	0.0174 (10)	0.0027 (10)
N4	0.0278 (12)	0.0226 (11)	0.0364 (13)	−0.0014 (9)	0.0127 (10)	0.0008 (9)
N5	0.0386 (14)	0.0235 (11)	0.0580 (16)	−0.0004 (11)	0.0257 (12)	−0.0021 (11)
N6	0.0340 (14)	0.0332 (13)	0.0579 (16)	0.0034 (11)	0.0222 (12)	−0.0018 (11)
C1	0.0237 (13)	0.0249 (13)	0.0252 (13)	−0.0014 (11)	0.0051 (11)	0.0005 (11)
C2	0.0345 (15)	0.0234 (13)	0.0378 (15)	−0.0019 (12)	0.0104 (12)	−0.0004 (11)
C3	0.0341 (16)	0.0282 (14)	0.0429 (16)	0.0073 (12)	0.0142 (13)	−0.0013 (12)
C4	0.0304 (15)	0.0365 (15)	0.0433 (17)	0.0050 (13)	0.0166 (14)	0.0024 (13)
C5	0.0262 (14)	0.0270 (14)	0.0408 (16)	−0.0008 (11)	0.0127 (12)	0.0046 (12)
C6	0.0269 (14)	0.0204 (13)	0.0301 (15)	−0.0008 (11)	0.0085 (12)	0.0019 (10)
C7	0.0287 (14)	0.0231 (12)	0.0282 (14)	−0.0015 (11)	0.0106 (12)	−0.0003 (10)
C8	0.0279 (14)	0.0226 (13)	0.0279 (14)	−0.0006 (11)	0.0097 (11)	0.0022 (11)
C9	0.0350 (16)	0.0233 (13)	0.0428 (16)	−0.0003 (12)	0.0156 (13)	−0.0003 (12)
C10	0.0337 (16)	0.0381 (16)	0.060 (2)	−0.0052 (13)	0.0225 (15)	0.0020 (14)
C11	0.0429 (18)	0.0256 (14)	0.073 (2)	−0.0053 (13)	0.0291 (17)	0.0016 (14)

Geometric parameters (Å, º)

Cu1—N1	2.027 (2)	C1—C2	1.377 (3)
Cu1—N2	1.969 (2)	C1—C6	1.461 (3)
Cu1—N1^{i}	2.027 (2)	C2—C3	1.376 (4)
Cu1—N2^{i}	1.969 (2)	C3—C4	1.377 (3)
N1—C1	1.354 (3)	C4—C5	1.376 (3)
N1—C5	1.341 (3)	C7—C8	1.468 (3)
N2—N3	1.366 (3)	C8—C9	1.394 (3)
N2—C6	1.343 (3)	C10—C11	1.371 (5)
N3—C7	1.334 (3)	C2—H2	0.9300
N4—C6	1.332 (3)	C3—H3	0.9300
N4—C7	1.360 (3)	C4—H4	0.9300
N5—C8	1.334 (3)	C5—H5	0.9300
N5—C11	1.337 (4)	C9—H9	0.9300
N6—C9	1.325 (4)	C10—H10	0.9300
N6—C10	1.332 (4)	C11—H11	0.9300
N1—Cu1—N2	81.43 (9)	N4—C6—C1	129.0 (2)
N1—Cu1—N1^{i}	180.00	N3—C7—N4	114.8 (2)
N1—Cu1—N2^{i}	98.58 (9)	N3—C7—C8	121.6 (2)
N1^{i}—Cu1—N2	98.58 (9)	N4—C7—C8	123.5 (2)
N2—Cu1—N2^{i}	180.00	N5—C8—C7	117.7 (2)
N1^{i}—Cu1—N2^{i}	81.43 (9)	N5—C8—C9	120.7 (2)
Cu1—N1—C1	113.74 (17)	C7—C8—C9	121.6 (2)
Cu1—N1—C5	128.07 (16)	N6—C9—C8	123.2 (2)
C1—N1—C5	118.0 (2)	N6—C10—C11	122.3 (3)
Cu1—N2—N3	139.18 (16)	N5—C11—C10	122.5 (3)
Cu1—N2—C6	113.69 (18)	C1—C2—H2	121.00
N3—N2—C6	106.66 (19)	C3—C2—H2	121.00
N2—N3—C7	104.0 (2)	C2—C3—H3	120.00

C6—N4—C7	100.83 (19)	C4—C3—H3	120.00
C8—N5—C11	116.0 (2)	C3—C4—H4	120.00
C9—N6—C10	115.3 (3)	C5—C4—H4	120.00
N1—C1—C2	122.4 (2)	N1—C5—H5	119.00
N1—C1—C6	112.9 (2)	C4—C5—H5	119.00
C2—C1—C6	124.7 (2)	N6—C9—H9	118.00
C1—C2—C3	118.7 (2)	C8—C9—H9	118.00
C2—C3—C4	119.4 (2)	N6—C10—H10	119.00
C3—C4—C5	119.1 (2)	C11—C10—H10	119.00
N1—C5—C4	122.4 (2)	N5—C11—H11	119.00
N2—C6—N4	113.6 (2)	C10—C11—H11	119.00
N2—C6—C1	117.4 (2)		

N2—Cu1—N1—C1	8.16 (18)	C7—N4—C6—N2	0.2 (3)
N2^{i}—Cu1—N1—C1	−171.84 (18)	C6—N4—C7—C8	177.0 (2)
N2—Cu1—N1—C5	−177.6 (2)	C8—N5—C11—C10	0.3 (4)
N2^{i}—Cu1—N1—C5	2.4 (2)	C11—N5—C8—C7	−178.3 (2)
N1—Cu1—N2—N3	−178.5 (3)	C11—N5—C8—C9	0.0 (4)
N1^{i}—Cu1—N2—N3	1.5 (3)	C9—N6—C10—C11	−0.5 (4)
N1—Cu1—N2—C6	−7.77 (18)	C10—N6—C9—C8	0.8 (4)
N1^{i}—Cu1—N2—C6	172.23 (18)	N1—C1—C6—N2	0.5 (3)
Cu1—N1—C5—C4	−172.0 (2)	N1—C1—C2—C3	0.4 (4)
C1—N1—C5—C4	2.1 (4)	C2—C1—C6—N4	1.1 (4)
Cu1—N1—C1—C2	172.57 (18)	C2—C1—C6—N2	−179.0 (2)
C5—N1—C1—C2	−2.3 (4)	N1—C1—C6—N4	−179.5 (2)
Cu1—N1—C1—C6	−6.9 (3)	C6—C1—C2—C3	179.8 (2)
C5—N1—C1—C6	178.2 (2)	C1—C2—C3—C4	1.7 (4)
N3—N2—C6—C1	−179.9 (2)	C2—C3—C4—C5	−2.0 (4)
Cu1—N2—C6—N4	−173.66 (17)	C3—C4—C5—N1	0.0 (4)
Cu1—N2—N3—C7	170.9 (2)	N3—C7—C8—N5	162.8 (2)
C6—N2—N3—C7	−0.2 (3)	N4—C7—C8—C9	167.4 (2)
N3—N2—C6—N4	0.0 (3)	N4—C7—C8—N5	−14.3 (4)
Cu1—N2—C6—C1	6.4 (3)	N3—C7—C8—C9	−15.5 (4)
N2—N3—C7—C8	−177.0 (2)	C7—C8—C9—N6	177.6 (2)
N2—N3—C7—N4	0.3 (3)	N5—C8—C9—N6	−0.6 (4)
C7—N4—C6—C1	−179.9 (2)	N6—C10—C11—N5	−0.1 (5)
C6—N4—C7—N3	−0.3 (3)		

Symmetry code: (i) −*x*+2, −*y*+2, −*z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···N5^{ii}	0.93	2.52	3.303 (3)	141
C5—H5···N3^{i}	0.93	2.39	3.169 (3)	141

Symmetry codes: (i) −*x*+2, −*y*+2, −*z*; (ii) −*x*+2, −*y*+1, −*z*.