trans,trans,trans-Diaquabis(nicotinamide-κN)bis(2-nitrobenzoato-κO)copper(II)

Kou-Lin Zhang,[a] Qiu-Lan Xie[a] and Seik Weng Ng[b]*

[a]College of Chemistry and Chemical Engineering, Yangzhou University, Yangzhou 225002, People's Republic of China, and [b]Department of Chemistry, University of Malaya, 50603, Kuala Lumpur, Malaysia
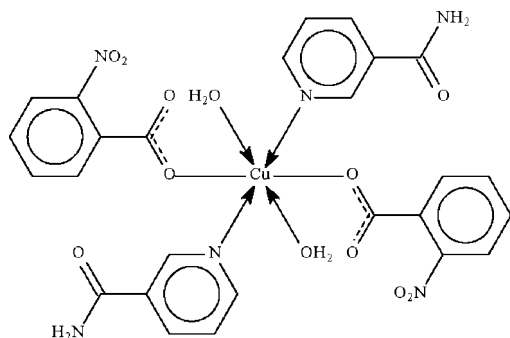
Correspondence e-mail: seikweng@um.edu.my

The water-coordinated metal atom in the title compound, $[Cu(C_7H_4NO_4)_2(C_6H_6N_2O)_2(H_2O)_2]$, lies on a center of inversion in an all-*trans* octahedral environment with slight distortions. The molecule interacts with adjacent molecules through O—H⋯O and N—H⋯O hydrogen bonds, forming a layered network parallel to (010).

Related literature

There are recent examples of diaquadi(arylcarboxylato)-di(nicotinamide)metal(II) compounds, see: Hökelek & Necefoğlu (2007a,b); Hökelek et al. (2007); Koksharova et al. (2006); Şahin et al. (2007a, 2007b); Stachova et al. (2006); Çaylak et al. (2007); Zhang et al. (2009).

Experimental

Crystal data

$[Cu(C_7H_4NO_4)_2(C_6H_6N_2O)_2(H_2O)_2]$	β = 104.012 (2)°
M_r = 676.05	V = 1423.63 (8) Å^3
Monoclinic, $P2_1/n$	Z = 2
a = 7.9582 (3) Å	Mo $K\alpha$ radiation
b = 18.7044 (6) Å	μ = 0.84 mm^{-1}
c = 9.8573 (2) Å	T = 295 K
	0.45 × 0.20 × 0.16 mm

Data collection

Bruker SMART area-detector diffractometer	7295 measured reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	2507 independent reflections
T_{min} = 0.557, T_{max} = 0.877	2069 reflections with $I > 2\sigma(I)$
	R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.111	
S = 1.12	$\Delta\rho_{max}$ = 0.31 e Å^{-3}
2507 reflections	$\Delta\rho_{min}$ = −0.46 e Å^{-3}
229 parameters	
4 restraints	

Table 1
Selected bond lengths (Å).

Cu1—O1	1.995 (2)	Cu1—O1w	2.537 (3)
Cu1—N2	2.006 (3)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O1w—H11⋯O2[i]	0.85 (4)	1.92 (2)	2.726 (4)	159 (4)
O1w—H12⋯O5[ii]	0.85 (4)	2.11 (2)	2.934 (2)	165 (3)
N3—H32⋯O2[iii]	0.85 (4)	2.15 (2)	2.929 (4)	152 (4)
N3—H31⋯O5[iv]	0.85 (4)	2.11 (2)	2.926 (4)	161 (4)

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x+1, y, z$; (iii) $x, y, z+1$; (iv) $-x, -y+1, -z+2$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

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metal-organic compounds

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Zhang, K.-L., Yang, B., Lin, J.-G. & Ng, S. W. (2009). *Acta Cryst.* E**65**, m292.

supporting information

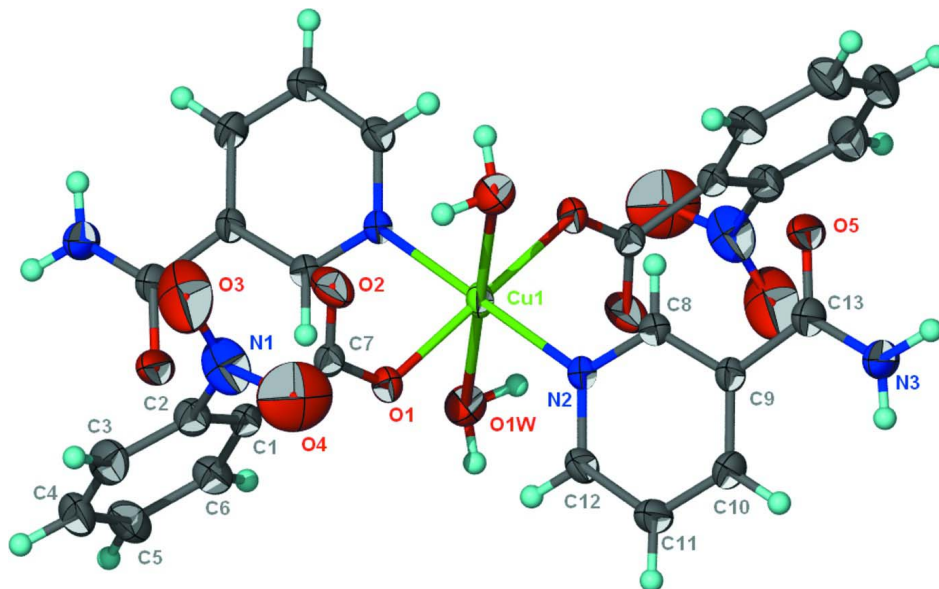# *trans,trans,trans*-Diaquabis(nicotinamide-*κN*)bis(2-nitrobenzoato-*κO*)copper(II)

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S1. Experimental

A water/methanol (1:1 *v/v*) solution (3 ml) of copper nitrate trihydrate (0.174 g, 0.6 mmol) was added to a water/methanol (1:1 *v/v*) solution (3 ml) of 2-nitrobenzoic acid (0.100 g, 0.6 mmol), sodium hydroxide (0.024 g 0.6 mmol) and nicotinamide (0.073 g, 0.6 mmol). Blue block were obtained after several days (yield: 40%). CH&N elemental analysis: calc. for $C_{26}H_{24}CuN_6O_{12}$: C 46.19, H 3.59, *N* 12.43%; found: C 46.37, H 3.41, N 12.60%.

S2. Refinement

Carbon-bound H atoms were placed in calculated positions and were allowed to ride on the parent atoms. The oxygen-bound ones were located in a difference Fourier map, and were refined with distance restraints N–H, O–H = 0.85±0.01 Å; an additional H···H 1.39 + 0.01 Å restraint was used. Their displacement parameters were freely refined.

Figure 1

Thermal ellipsoid plot of $Cu(H_2O)_2(C_7H_4NO_4)_2(C_6H_6N_2O)_2$; displacement ellipsoids are drawn at the 50% probabability level, and H atoms as spheres of arbitrary radii.

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$M_r = 676.05$	Hall symbol: -P 2yn

$a = 7.9582 (3)$ Å
$b = 18.7044 (6)$ Å
$c = 9.8573 (2)$ Å
$\beta = 104.012 (2)°$
$V = 1423.63 (8)$ Å^3
$Z = 2$
$F(000) = 694$
$D_x = 1.577$ Mg m^{-3}

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3858 reflections
$\theta = 2.2–25.0°$
$\mu = 0.84$ mm^{-1}
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Block, blue
$0.45 \times 0.20 \times 0.16$ mm

Data collection

Bruker SMART area-detector
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Radiation source: medium-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan
  (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.557$, $T_{max} = 0.877$

7295 measured reflections
2507 independent reflections
2069 reflections with $I > 2\sigma(I)$
$R_{int} = 0.036$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.2°$
$h = -9 \rightarrow 9$
$k = -14 \rightarrow 22$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.111$
$S = 1.12$
2507 reflections
229 parameters
4 restraints
Primary atom site location: structure-invariant
  direct methods

Secondary atom site location: difference Fourier
  map
Hydrogen site location: inferred from
  neighbouring sites
H atoms treated by a mixture of independent
  and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0395P)^2 + 1.8061P]$
  where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.46$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.5000	0.5000	0.5000	0.02960 (19)
O1	0.6141 (3)	0.41263 (12)	0.4483 (2)	0.0329 (5)
O2	0.3896 (3)	0.37179 (15)	0.2856 (3)	0.0531 (7)
O3	0.3215 (5)	0.2416 (3)	0.0916 (5)	0.1123 (16)
O4	0.3942 (5)	0.2153 (2)	0.3108 (5)	0.1137 (16)
O5	0.0632 (4)	0.49124 (18)	0.8331 (3)	0.0642 (9)
O1W	0.8082 (4)	0.54476 (16)	0.5876 (3)	0.0493 (7)
H11	0.772 (6)	0.5753 (19)	0.637 (4)	0.067 (15)*
H12	0.883 (5)	0.522 (2)	0.647 (4)	0.073 (16)*
N1	0.4256 (5)	0.2375 (2)	0.2043 (5)	0.0624 (10)
N2	0.4917 (3)	0.45491 (14)	0.6829 (3)	0.0290 (6)
N3	0.1614 (5)	0.4274 (2)	1.0283 (3)	0.0539 (9)
H31	0.081 (4)	0.442 (2)	1.065 (4)	0.069 (14)*
H32	0.241 (4)	0.403 (2)	1.082 (4)	0.075 (16)*
C1	0.6639 (4)	0.32322 (17)	0.2924 (3)	0.0297 (7)
C2	0.6033 (5)	0.26281 (19)	0.2137 (4)	0.0372 (8)
C3	0.7038 (6)	0.2231 (2)	0.1461 (4)	0.0496 (10)

H3	0.6578	0.1835	0.0929	0.057 (12)*
C4	0.8740 (6)	0.2428 (2)	0.1585 (4)	0.0552 (11)
H4	0.9433	0.2170	0.1125	0.065 (13)*
C5	0.9406 (5)	0.3009 (2)	0.2392 (4)	0.0503 (10)
H5	1.0561	0.3135	0.2495	0.067 (14)*
C6	0.8366 (4)	0.3409 (2)	0.3053 (4)	0.0395 (8)
H6	0.8834	0.3801	0.3591	0.038 (10)*
C7	0.5449 (4)	0.37176 (17)	0.3480 (3)	0.0289 (7)
C8	0.3508 (4)	0.46333 (17)	0.7327 (3)	0.0306 (7)
H8	0.2571	0.4882	0.6785	0.029 (9)*
C9	0.3378 (4)	0.43678 (18)	0.8613 (3)	0.0304 (7)
C10	0.4781 (5)	0.3999 (2)	0.9403 (4)	0.0434 (9)
H10	0.4747	0.3819	1.0276	0.048 (11)*
C11	0.6240 (5)	0.3899 (2)	0.8889 (4)	0.0461 (10)
H11A	0.7186	0.3644	0.9402	0.062 (13)*
C12	0.6259 (4)	0.41833 (19)	0.7608 (4)	0.0364 (8)
H12A	0.7241	0.4120	0.7268	0.032 (9)*
C13	0.1760 (5)	0.4530 (2)	0.9067 (4)	0.0419 (9)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0375 (3)	0.0296 (3)	0.0256 (3)	0.0041 (3)	0.0153 (2)	0.0014 (2)
O1	0.0378 (13)	0.0332 (12)	0.0292 (12)	0.0057 (10)	0.0110 (10)	−0.0034 (10)
O2	0.0318 (14)	0.0677 (19)	0.0557 (17)	0.0093 (13)	0.0028 (12)	−0.0203 (14)
O3	0.061 (2)	0.178 (5)	0.091 (3)	−0.027 (3)	0.006 (2)	−0.071 (3)
O4	0.094 (3)	0.118 (4)	0.140 (4)	−0.030 (3)	0.049 (3)	0.048 (3)
O5	0.0489 (16)	0.107 (3)	0.0436 (15)	0.0375 (17)	0.0254 (13)	0.0285 (16)
O1W	0.0454 (16)	0.0586 (19)	0.0407 (16)	0.0032 (14)	0.0045 (13)	−0.0056 (14)
N1	0.060 (2)	0.051 (2)	0.079 (3)	−0.0141 (19)	0.023 (2)	−0.022 (2)
N2	0.0302 (14)	0.0338 (15)	0.0250 (14)	0.0037 (12)	0.0104 (11)	−0.0004 (12)
N3	0.046 (2)	0.084 (3)	0.039 (2)	0.020 (2)	0.0237 (17)	0.0225 (18)
C1	0.0332 (18)	0.0310 (17)	0.0259 (17)	0.0033 (14)	0.0089 (14)	0.0021 (14)
C2	0.040 (2)	0.0354 (19)	0.037 (2)	0.0021 (16)	0.0110 (16)	0.0003 (16)
C3	0.066 (3)	0.037 (2)	0.046 (2)	0.007 (2)	0.014 (2)	−0.0094 (18)
C4	0.069 (3)	0.054 (3)	0.050 (3)	0.025 (2)	0.027 (2)	0.003 (2)
C5	0.041 (2)	0.052 (2)	0.062 (3)	0.0077 (19)	0.0224 (19)	0.005 (2)
C6	0.036 (2)	0.037 (2)	0.045 (2)	0.0019 (16)	0.0094 (16)	−0.0030 (17)
C7	0.0341 (18)	0.0287 (17)	0.0254 (17)	0.0025 (14)	0.0104 (14)	0.0028 (14)
C8	0.0326 (18)	0.0327 (18)	0.0270 (17)	0.0055 (15)	0.0082 (14)	0.0006 (14)
C9	0.0335 (18)	0.0333 (18)	0.0269 (17)	0.0033 (14)	0.0123 (14)	0.0022 (14)
C10	0.050 (2)	0.054 (2)	0.0303 (18)	0.0127 (19)	0.0168 (17)	0.0124 (17)
C11	0.043 (2)	0.056 (2)	0.042 (2)	0.0189 (19)	0.0159 (18)	0.0153 (18)
C12	0.0342 (19)	0.041 (2)	0.038 (2)	0.0087 (16)	0.0168 (16)	0.0057 (16)
C13	0.042 (2)	0.053 (2)	0.0347 (19)	0.0079 (18)	0.0167 (17)	0.0081 (17)

Geometric parameters (Å, º)

Cu1—O1i	1.995 (2)	C1—C6	1.389 (5)
Cu1—O1	1.995 (2)	C1—C7	1.507 (4)
Cu1—N2i	2.006 (3)	C2—C3	1.377 (5)
Cu1—N2	2.006 (3)	C3—C4	1.380 (6)
Cu1—O1w	2.537 (3)	C3—H3	0.9300
O1—C7	1.266 (4)	C4—C5	1.375 (6)
O2—C7	1.240 (4)	C4—H4	0.9300
O3—N1	1.216 (5)	C5—C6	1.389 (5)
O4—N1	1.210 (5)	C5—H5	0.9300
O5—C13	1.237 (4)	C6—H6	0.9300
O1W—H11	0.85 (4)	C8—C9	1.389 (4)
O1W—H12	0.85 (4)	C8—H8	0.9300
N1—C2	1.472 (5)	C9—C10	1.381 (5)
N2—C8	1.337 (4)	C9—C13	1.493 (5)
N2—C12	1.342 (4)	C10—C11	1.387 (5)
N3—C13	1.322 (5)	C10—H10	0.9300
N3—H31	0.85 (4)	C11—C12	1.374 (5)
N3—H32	0.85 (4)	C11—H11A	0.9300
C1—C2	1.389 (5)	C12—H12A	0.9300
O1i—Cu1—O1	180.000 (1)	C4—C3—H3	120.5
O1i—Cu1—N2i	90.07 (10)	C5—C4—C3	119.7 (4)
O1—Cu1—N2i	89.93 (10)	C5—C4—H4	120.1
O1i—Cu1—N2	89.93 (10)	C3—C4—H4	120.1
O1—Cu1—N2	90.07 (10)	C4—C5—C6	120.4 (4)
N2i—Cu1—N2	180.00 (14)	C4—C5—H5	119.8
O1i—Cu1—O1W	96.04 (9)	C6—C5—H5	119.8
O1—Cu1—O1W	83.96 (9)	C5—C6—C1	121.2 (4)
N2i—Cu1—O1W	85.84 (10)	C5—C6—H6	119.4
N2—Cu1—O1W	94.16 (10)	C1—C6—H6	119.4
C7—O1—Cu1	123.7 (2)	O2—C7—O1	125.5 (3)
Cu1—O1W—H11	89 (3)	O2—C7—C1	117.3 (3)
Cu1—O1W—H12	122 (3)	O1—C7—C1	117.1 (3)
H11—O1W—H12	103 (4)	N2—C8—C9	123.2 (3)
O4—N1—O3	125.1 (4)	N2—C8—H8	118.4
O4—N1—C2	116.9 (4)	C9—C8—H8	118.4
O3—N1—C2	117.9 (4)	C10—C9—C8	117.7 (3)
C8—N2—C12	118.1 (3)	C10—C9—C13	124.8 (3)
C8—N2—Cu1	119.6 (2)	C8—C9—C13	117.5 (3)
C12—N2—Cu1	122.3 (2)	C9—C10—C11	119.7 (3)
C13—N3—H31	120 (3)	C9—C10—H10	120.2
C13—N3—H32	123 (3)	C11—C10—H10	120.2
H31—N3—H32	115 (4)	C12—C11—C10	118.7 (3)
C2—C1—C6	116.5 (3)	C12—C11—H11A	120.7
C2—C1—C7	122.0 (3)	C10—C11—H11A	120.7
C6—C1—C7	121.2 (3)	N2—C12—C11	122.6 (3)

C3—C2—C1	123.1 (3)	N2—C12—H12A	118.7
C3—C2—N1	117.2 (3)	C11—C12—H12A	118.7
C1—C2—N1	119.7 (3)	O5—C13—N3	122.1 (3)
C2—C3—C4	119.0 (4)	O5—C13—C9	119.9 (3)
C2—C3—H3	120.5	N3—C13—C9	118.0 (3)
N2^i—Cu1—O1—C7	−65.5 (2)	C2—C1—C6—C5	1.7 (5)
N2—Cu1—O1—C7	114.5 (2)	C7—C1—C6—C5	−171.9 (3)
O1W—Cu1—O1—C7	−151.3 (2)	Cu1—O1—C7—O2	−14.1 (5)
O1^i—Cu1—N2—C8	40.3 (2)	Cu1—O1—C7—C1	160.6 (2)
O1—Cu1—N2—C8	−139.7 (2)	C2—C1—C7—O2	−24.1 (5)
O1W—Cu1—N2—C8	136.3 (2)	C6—C1—C7—O2	149.2 (3)
O1^i—Cu1—N2—C12	−137.2 (3)	C2—C1—C7—O1	160.7 (3)
O1—Cu1—N2—C12	42.8 (3)	C6—C1—C7—O1	−26.0 (4)
O1W—Cu1—N2—C12	−41.1 (3)	C12—N2—C8—C9	0.7 (5)
C6—C1—C2—C3	−2.6 (5)	Cu1—N2—C8—C9	−176.9 (2)
C7—C1—C2—C3	171.0 (3)	N2—C8—C9—C10	−0.1 (5)
C6—C1—C2—N1	175.3 (3)	N2—C8—C9—C13	177.3 (3)
C7—C1—C2—N1	−11.1 (5)	C8—C9—C10—C11	−0.8 (6)
O4—N1—C2—C3	111.8 (5)	C13—C9—C10—C11	−178.0 (4)
O3—N1—C2—C3	−69.5 (5)	C9—C10—C11—C12	1.2 (6)
O4—N1—C2—C1	−66.2 (5)	C8—N2—C12—C11	−0.4 (5)
O3—N1—C2—C1	112.5 (4)	Cu1—N2—C12—C11	177.2 (3)
C1—C2—C3—C4	1.3 (6)	C10—C11—C12—N2	−0.6 (6)
N1—C2—C3—C4	−176.6 (4)	C10—C9—C13—O5	174.3 (4)
C2—C3—C4—C5	0.9 (6)	C8—C9—C13—O5	−2.9 (5)
C3—C4—C5—C6	−1.6 (6)	C10—C9—C13—N3	−3.5 (6)
C4—C5—C6—C1	0.3 (6)	C8—C9—C13—N3	179.3 (4)

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···A	D—H	H···A	D···A	D—H···A
O1w—H11···O2^i	0.85 (4)	1.92 (2)	2.726 (4)	159 (4)
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N3—H32···O2^{iii}	0.85 (4)	2.15 (2)	2.929 (4)	152 (4)
N3—H31···O5^{iv}	0.85 (4)	2.11 (2)	2.926 (4)	161 (4)

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