Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis(2-chlorobenzoato-κO)bis(1-vinylimidazole-κN^3)copper(II)

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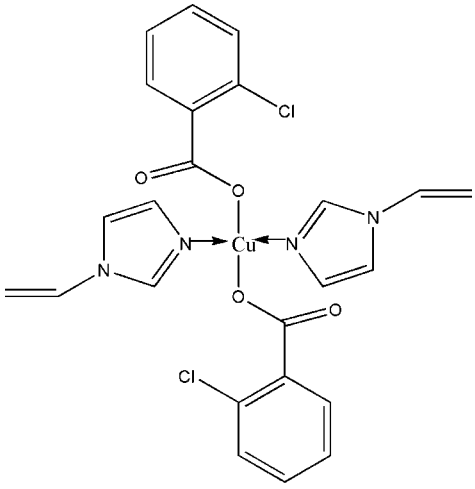
Received 14 September 2008; accepted 19 September 2008

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.011 Å; R factor = 0.073; wR factor = 0.192; data-to-parameter ratio = 13.7.

In the title compound, $[Cu(C_7H_4ClO_2)_2(C_5H_6N_2)_2]$, each Cu^{II} ion, located on an inversion center, has a slightly distorted square-planar coordination geometry formed by two 1-vinylimidazole molecules [Cu—N = 1.954 (6) Å] and two 2-chlorobenzoate anions [Cu—O = 1.958 (6) Å]. Weak intermolecular C—H···O hydrogen bonds contribute to the crystal packing stability.

Related literature

A square-planar coordination environment of Cu^{II} was also observed in bis(3-hydroxybenzoato-κO)bis(1H-imidazole-κN^3)copper(II), see: Liu *et al.* (2006).



Experimental

Crystal data

$[Cu(C_7H_4ClO_2)_2(C_5H_6N_2)_2]$
M_r = 562.89
Monoclinic, $P2_1/c$
a = 7.9360 (16) Å
b = 11.236 (2) Å
c = 14.190 (3) Å
β = 104.36 (3)°
V = 1225.8 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.15 mm^{-1}
T = 293 (2) K
0.20 × 0.10 × 0.10 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.803, T_{max} = 0.894
2204 measured reflections
2115 independent reflections
1620 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.073
$wR(F^2)$ = 0.192
S = 1.04
2115 reflections
154 parameters
49 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.73 e Å^{-3}
$\Delta\rho_{min}$ = −0.89 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1A···O2^{i}	0.93	2.56	3.484 (10)	174
C3—H3A···O1^{ii}	0.93	2.49	2.918 (8)	108
C5—H5A···O2^{i}	0.93	2.45	3.342 (9)	160
C11—H11A···O2^{iii}	0.93	2.60	3.460 (9)	155

Symmetry codes: (i) $x-1, y, z$; (ii) $-x, -y, -z$; (iii) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and local programs.

This work was supported by the National Natural Science Foundation of China (grant No. 20601015) and the Natural Science Foundation of Shandong Province (Y2006B12).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2449).

References

Bruker (2001). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
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Sheldrick, G. M. (2004). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2008). E**64**, m1321 [doi:10.1107/S1600536808030237]

Bis(2-chlorobenzoato-κO)bis(1-vinylimidazole-κN^3)copper(II)

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S1. Comment

In the title compound, (I) (Fig. 1), each Cu ion is coordinated by a pair of 1-vinylimidazole ligands and a pair of monodentate carboxylate groups, affording a square planar N_2O_2 coordination geometry. The CuN_2O_2 core involving the central atoms is almost perfectly square planar. The *trans* angles are all 180° for symmetry requirements and the *cis* ones are 89.52 (19)° and 90.48 (19)° for N—Cu—O, respectively. The Cu—*N*(imidazole) distance is 1.954 (6)Å and The Cu—O bond distance is 1.958 (4) Å. These bond distances are comparable with the reported data (Liu *et al.*, 2006). The five atoms of CuN_2O_2 are coplanar. Distances and angles in 1-vinylimidazole are normal. The weak intermolecular C—H···O interactions (Table 1) stabilize the structure.

S2. Experimental

Copper(II) acetate hydrate(2.00 g, 10 mmol), 1-vinylimidazole(0.99 g, 10 mmol) and 2-chlorobenzoic acid(1.55 g, 10 mmol) were dissolved in water(40 ml). The pH of the solution was adjusted to 7 with 0.2*M* sodium hydroxide. The solution was filtered; blue single crystals of (I) were isolated after several days.

S3. Refinement

H atoms were positioned geometrically (C—H = 0.93 Å) and allowed to ride on their parent atoms with U_{iso}(H) = 1.2 U_{eq}(C).

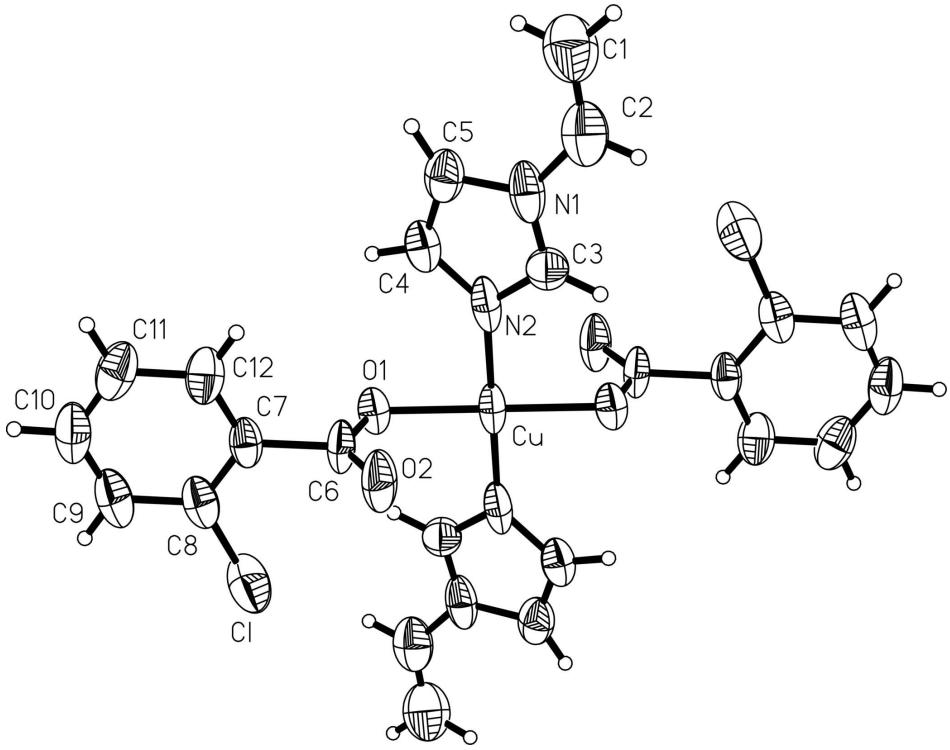

Figure 1

The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. The unlabelled atoms are related with the labelled ones by symmetry operation (-*x*, -*y*, -*z*).

Bis(2-chlorobenzoato-κO)bis(1-vinylimidazole-κN^3)copper(II)

Crystal data

$[Cu(C_7H_4ClO_2)_2(C_5H_6N_2)_2]$
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Hall symbol: -P 2ybc
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c = 14.190 (3) Å
β = 104.36 (3)°
V = 1225.8 (5) Å^3
Z = 2
$F(000)$ = 574
D_x = 1.525 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 25 reflections
θ = 10–14°
μ = 1.15 mm^{-1}
T = 293 K
Block, blue
0.20 × 0.10 × 0.10 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Thin–slice ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.803, T_{max} = 0.894
2204 measured reflections
2115 independent reflections
1620 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 25.2°, θ_{min} = 2.3°
h = −9→9
k = 0→13
l = 0→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.073$
$wR(F^2) = 0.192$
$S = 1.04$
2115 reflections
154 parameters
49 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
$w = 1/[\sigma^2(F_o^2) + (0.07P)^2 + 6P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.73$ e Å^{-3}
$\Delta\rho_{min} = -0.89$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu	0.0000	0.0000	0.0000	0.0439 (4)
Cl	0.3736 (3)	−0.36078 (18)	0.02395 (17)	0.0794 (6)
O1	0.0066 (5)	−0.1740 (3)	0.0077 (3)	0.0455 (10)
N1	−0.3796 (8)	0.0695 (5)	0.1425 (4)	0.0550 (14)
C1	−0.6165 (13)	0.1373 (8)	0.2115 (6)	0.088 (3)
H1A	−0.6754	0.0655	0.1961	0.105*
H1B	−0.6638	0.1972	0.2422	0.105*
O2	0.1925 (7)	−0.1406 (4)	0.1509 (3)	0.0647 (14)
N2	−0.1911 (7)	0.0008 (4)	0.0642 (4)	0.0527 (14)
C2	−0.4664 (11)	0.1540 (7)	0.1896 (5)	0.066 (2)
H2A	−0.4120	0.2270	0.2063	0.079*
C3	−0.2436 (8)	0.0933 (6)	0.1068 (5)	0.047
H3A	−0.1907	0.1676	0.1114	0.057*
C4	−0.3049 (9)	−0.0881 (6)	0.0741 (5)	0.0504 (15)
H4A	−0.3010	−0.1654	0.0513	0.060*
C5	−0.4234 (9)	−0.0489 (6)	0.1212 (5)	0.0537 (16)
H5A	−0.5138	−0.0917	0.1360	0.064*
C6	0.1057 (9)	−0.2068 (5)	0.0889 (5)	0.0501 (16)
C7	0.1031 (8)	−0.3403 (5)	0.1088 (4)	0.0433 (13)
C8	0.2177 (9)	−0.4153 (6)	0.0813 (4)	0.0513 (15)
C9	0.2146 (11)	−0.5370 (6)	0.0999 (6)	0.0662 (19)
H9A	0.2926	−0.5882	0.0812	0.079*
C10	0.0945 (11)	−0.5801 (6)	0.1461 (6)	0.0676 (19)
H10A	0.0906	−0.6613	0.1580	0.081*
C11	−0.0196 (11)	−0.5057 (7)	0.1749 (5)	0.0648 (18)

H11A	−0.0990	−0.5360	0.2071	0.078*
C12	−0.0162 (10)	−0.3853 (6)	0.1558 (5)	0.0580 (17)
H12A	−0.0943	−0.3344	0.1746	0.070*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu	0.0696 (7)	0.0204 (5)	0.0350 (5)	0.0026 (5)	0.0001 (5)	0.0014 (4)
Cl	0.1031 (15)	0.0558 (11)	0.0838 (14)	0.0230 (11)	0.0319 (12)	0.0061 (10)
O1	0.060 (2)	0.030 (2)	0.043 (2)	0.0052 (19)	0.0066 (19)	0.0033 (18)
N1	0.088 (4)	0.033 (3)	0.035 (3)	0.009 (3)	−0.004 (3)	0.002 (2)
C1	0.115 (7)	0.071 (6)	0.079 (6)	0.004 (5)	0.029 (6)	−0.011 (5)
O2	0.094 (4)	0.029 (2)	0.058 (3)	−0.003 (2)	−0.006 (3)	−0.009 (2)
N2	0.075 (3)	0.024 (2)	0.048 (3)	0.008 (3)	−0.008 (3)	0.001 (2)
C2	0.096 (6)	0.054 (5)	0.042 (4)	0.004 (4)	0.004 (4)	0.007 (3)
C3	0.047	0.047	0.047	0.000	0.012	0.000
C4	0.068 (4)	0.035 (3)	0.043 (3)	0.008 (3)	0.006 (3)	0.003 (3)
C5	0.067 (4)	0.043 (3)	0.045 (4)	−0.001 (3)	0.001 (3)	0.009 (3)
C6	0.074 (4)	0.020 (3)	0.050 (4)	−0.004 (3)	0.004 (3)	0.000 (3)
C7	0.064 (3)	0.028 (3)	0.031 (3)	0.002 (2)	−0.001 (2)	−0.002 (2)
C8	0.072 (4)	0.037 (3)	0.040 (3)	0.011 (3)	0.004 (3)	−0.002 (3)
C9	0.091 (5)	0.039 (3)	0.062 (4)	0.017 (3)	0.008 (4)	−0.001 (3)
C10	0.091 (5)	0.035 (3)	0.063 (4)	−0.005 (3)	−0.007 (3)	0.007 (3)
C11	0.086 (4)	0.053 (4)	0.051 (4)	−0.017 (3)	0.010 (3)	0.013 (3)
C12	0.085 (4)	0.042 (3)	0.047 (3)	−0.002 (3)	0.017 (3)	0.007 (3)

Geometric parameters (Å, º)

Cu—N2^{i}	1.954 (6)	C3—H3A	0.9300
Cu—N2	1.954 (6)	C4—C5	1.356 (9)
Cu—O1^{i}	1.958 (4)	C4—H4A	0.9300
Cu—O1	1.958 (4)	C5—H5A	0.9300
Cl—C8	1.751 (7)	C6—C7	1.528 (8)
O1—C6	1.278 (7)	C7—C8	1.366 (8)
N1—C3	1.327 (8)	C7—C12	1.383 (9)
N1—C5	1.389 (9)	C8—C9	1.394 (10)
N1—C2	1.433 (9)	C9—C10	1.372 (11)
C1—C2	1.317 (10)	C9—H9A	0.9300
C1—H1A	0.9300	C10—C11	1.367 (11)
C1—H1B	0.9300	C10—H10A	0.9300
O2—C6	1.225 (7)	C11—C12	1.381 (9)
N2—C3	1.320 (8)	C11—H11A	0.9300
N2—C4	1.377 (8)	C12—H12A	0.9300
C2—H2A	0.9300		
N2^{i}—Cu—N2	180.0 (3)	C4—C5—N1	104.5 (6)
N2^{i}—Cu—O1^{i}	89.52 (19)	C4—C5—H5A	127.7
N2—Cu—O1^{i}	90.48 (19)	N1—C5—H5A	127.7

N2^{i}—Cu—O1	90.48 (19)	O2—C6—O1	125.6 (5)
N2—Cu—O1	89.52 (19)	O2—C6—C7	119.7 (6)
O1^{i}—Cu—O1	180.0 (4)	O1—C6—C7	114.6 (5)
C6—O1—Cu	109.9 (4)	C8—C7—C12	119.8 (6)
C3—N1—C5	107.1 (6)	C8—C7—C6	120.9 (6)
C3—N1—C2	125.1 (6)	C12—C7—C6	119.4 (6)
C5—N1—C2	127.8 (6)	C7—C8—C9	120.4 (7)
C2—C1—H1A	120.0	C7—C8—Cl	120.9 (5)
C2—C1—H1B	120.0	C9—C8—Cl	118.6 (5)
H1A—C1—H1B	120.0	C10—C9—C8	118.9 (7)
C3—N2—C4	103.6 (6)	C10—C9—H9A	120.5
C3—N2—Cu	125.9 (4)	C8—C9—H9A	120.5
C4—N2—Cu	130.4 (4)	C11—C10—C9	121.1 (7)
C1—C2—N1	125.6 (8)	C11—C10—H10A	119.4
C1—C2—H2A	117.2	C9—C10—H10A	119.4
N1—C2—H2A	117.2	C10—C11—C12	119.6 (7)
N2—C3—N1	113.2 (6)	C10—C11—H11A	120.2
N2—C3—H3A	123.4	C12—C11—H11A	120.2
N1—C3—H3A	123.4	C11—C12—C7	120.1 (7)
C5—C4—N2	111.6 (6)	C11—C12—H12A	119.9
C5—C4—H4A	124.2	C7—C12—H12A	119.9
N2—C4—H4A	124.2		

N2^{i}—Cu—O1—C6	92.5 (4)	Cu—O1—C6—O2	−4.0 (9)
N2—Cu—O1—C6	−87.5 (4)	Cu—O1—C6—C7	172.6 (4)
O1^{i}—Cu—N2—C3	−17.5 (5)	O2—C6—C7—C8	−92.3 (8)
O1—Cu—N2—C3	162.5 (5)	O1—C6—C7—C8	90.9 (7)
O1^{i}—Cu—N2—C4	160.1 (5)	O2—C6—C7—C12	87.2 (8)
O1—Cu—N2—C4	−19.9 (5)	O1—C6—C7—C12	−89.6 (7)
C3—N1—C2—C1	168.6 (8)	C12—C7—C8—C9	0.4 (10)
C5—N1—C2—C1	−8.3 (11)	C6—C7—C8—C9	179.9 (6)
C4—N2—C3—N1	0.2 (7)	C12—C7—C8—Cl	−178.6 (5)
Cu—N2—C3—N1	178.3 (4)	C6—C7—C8—Cl	0.9 (8)
C5—N1—C3—N2	−0.6 (7)	C7—C8—C9—C10	0.1 (10)
C2—N1—C3—N2	−178.0 (5)	Cl—C8—C9—C10	179.0 (6)
C3—N2—C4—C5	0.3 (7)	C8—C9—C10—C11	−0.8 (11)
Cu—N2—C4—C5	−177.7 (4)	C9—C10—C11—C12	1.1 (11)
N2—C4—C5—N1	−0.7 (7)	C10—C11—C12—C7	−0.7 (11)
C3—N1—C5—C4	0.8 (7)	C8—C7—C12—C11	0.0 (10)
C2—N1—C5—C4	178.0 (6)	C6—C7—C12—C11	−179.6 (6)

Symmetry code: (i) −*x*, −*y*, −*z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*A*···O2^{ii}	0.93	2.56	3.484 (10)	174
C3—H3*A*···O1^{i}	0.93	2.49	2.918 (8)	108

C5—H5*A*···O2^{ii}	0.93	2.45	3.342 (9)	160
C11—H11*A*···O2^{iii}	0.93	2.60	3.460 (9)	155

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