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{1,1′-[*o*-Phenylenebis(nitrilomethylidyne)]di-2-naphtholato}copper(II)

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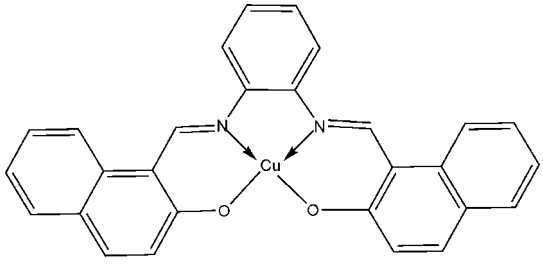
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.007 Å; R factor = 0.057; wR factor = 0.102; data-to-parameter ratio = 11.9.

In the title complex, $[Cu(C_{28}H_{18}N_2O_2)]$, the Cu^{II} atom is coordinated by two N [Cu—N = 1.913 (4) and 1.919 (4) Å] and two O [Cu—O = 1.872 (3) and 1.880 (3) Å] atoms from the *o*-phenylenebis(naphthalideneamine) ligand in a distorted square-planar geometry. Molecules related by centres of symmetry separated by a *b*/2 translation form stacks along the *b* axis with shortest C···C distances of 3.284 (8) and 3.298 (7) Å. In these stacks, short Cu···Cu distances of 3.446 (3) Å are also observed in alternating pairs of molecules.

Related literature

For the general role of Schiff bases, see: Gamovski *et al.* (1993). For crystal structures of related complexes, see: MacLachlan *et al.* (1996).



Experimental

Crystal data

$[Cu(C_{28}H_{18}N_2O_2)]$
M_r = 477.98
Monoclinic, $P2_1/n$
a = 16.019 (13) Å
b = 7.764 (6) Å
c = 16.334 (14) Å
β = 97.042 (13)°
V = 2016 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.12 mm^{-1}
T = 298 (2) K
0.42 × 0.12 × 0.05 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.652, T_{max} = 0.946
8028 measured reflections
3534 independent reflections
2081 reflections with $I > 2\sigma(I)$
R_{int} = 0.082

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.102
S = 1.00
3534 reflections
298 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O1^{i}	0.93	2.52	3.326 (6)	145

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2271).

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supplementary materials

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{1,1'-[*o*-Phenylenebis(nitrilomethylidyne)]di-2-naphtholato}copper(II)

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Comment

Schiff base complexes play an important role in coordination chemistry (Gamovski *et al.*, 1993). In a continuation of a study of Schiff base ligands and their copper(II) complexes, we report here the title complex (Fig. 1), in which the Cu atom exists in a squareplanar geometry with the max deviation from the mean plane of 0.0713 Å. The Cu—N and Cu—O bond lengths are comparable to those observed in other copper(II) complexes (MacLachlan *et al.*, 1996).

In the crystal, the molecules related by the centres of symmetry separated by the b/2 translation form stacks along the *b* axis with the short intermolecular distances C2···C20^{ii} and C2···C12^{iii} of 3.284 (8) and 3.298 (7) Å, respectively [symmetry codes: (ii) −*x*, 2 − *y*, −*z*; (iii) −*x*, 1 − *y*, −*z*]. In these stacks, the short Cu···Cu^{iii} distances of 3.446 (3) Å are also observed in alternating pairs of the molecules. The weak intermolecular C—H···O hydrogen bonds (Table) contribute to the further packing stabilization.

Experimental

o-Phenylenediamine(0.5 mmol, 54.11 mg) was dissolved in hot methanol (10 ml) and added dropwise to a methanol solution (5 ml) of 2- hydroxy-1-naphthaldehyde (1 mmol, 172.19 mg). The mixture was then stirred at 323 K for 2 h. An aqueous solution (2 ml) of copper(II) acetate hydrate (0.5 mmol, 99.86 mg) was then added dropwise and the mixture stirred for another 5 h. The solution was held at room temperature for about one week, whereupon red prism-shaped crystals suitable for X-ray diffraction analysis were obtained.

Refinement

All H atoms were placed in geometrically idealized positions (C—H 0.93 Å) and treated as riding on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C).

Figures

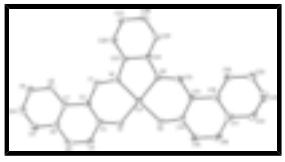


Fig. 1. The molecular structure of (I), with atom labels and 30% probability displacement ellipsoids for non-H atoms.

{1,1'-[*o*-Phenylenebis(nitrilomethylidyne)]di-2-naphtholato}copper(II)

Crystal data

$[Cu(C_{28}H_{18}N_2O_2)]$ F_{000} = 980

M_r = 477.98	D_x = 1.575 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 16.019 (13) Å	Cell parameters from 2054 reflections
b = 7.764 (6) Å	θ = 2.9–27.9º
c = 16.334 (14) Å	μ = 1.12 mm^{-1}
β = 97.042 (13)º	T = 298 (2) K
V = 2016 (3) Å^3	Prism, red
Z = 4	0.42 × 0.12 × 0.05 mm

Data collection

Bruker SMART CCD area-detector diffractometer	3534 independent reflections
Radiation source: fine-focus sealed tube	2081 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.082
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −18→19
T_{min} = 0.652, T_{max} = 0.946	k = −9→9
8028 measured reflections	l = −8→19

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.057	H-atom parameters constrained
$wR(F^2)$ = 0.102	$w = 1/[\sigma^2(F_o^2) + (0.0237P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.00	$(\Delta/\sigma)_{max} < 0.001$
3534 reflections	$\Delta\rho_{max}$ = 0.33 e Å^{-3}
298 parameters	$\Delta\rho_{min}$ = −0.42 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.04588 (3)	0.67783 (8)	0.05014 (3)	0.03463 (19)
N1	−0.0368 (2)	0.5873 (5)	0.1135 (2)	0.0304 (10)
N2	−0.0482 (2)	0.7732 (5)	−0.0191 (2)	0.0311 (10)
O1	0.13543 (17)	0.5793 (4)	0.11874 (18)	0.0366 (9)
O2	0.12563 (17)	0.7745 (4)	−0.01174 (18)	0.0431 (10)
C1	−0.0211 (3)	0.5039 (7)	0.1831 (3)	0.0336 (12)
H1	−0.0671	0.4732	0.2097	0.040*
C2	0.0598 (3)	0.4557 (6)	0.2222 (3)	0.0319 (12)
C3	0.1330 (3)	0.4951 (6)	0.1868 (3)	0.0328 (12)
C4	0.2121 (3)	0.4396 (7)	0.2281 (3)	0.0432 (14)
H4	0.2605	0.4608	0.2036	0.052*
C5	0.2192 (3)	0.3577 (7)	0.3012 (3)	0.0412 (14)
H5	0.2722	0.3265	0.3265	0.049*
C6	0.1477 (3)	0.3183 (7)	0.3404 (3)	0.0356 (12)
C7	0.0668 (3)	0.3674 (6)	0.3018 (3)	0.0333 (12)
C8	−0.0016 (3)	0.3251 (8)	0.3444 (3)	0.0448 (13)
H8	−0.0557	0.3546	0.3213	0.054*
C9	0.0089 (3)	0.2416 (7)	0.4192 (3)	0.0552 (17)
H9	−0.0375	0.2170	0.4463	0.066*
C10	0.0890 (3)	0.1940 (8)	0.4543 (3)	0.0519 (15)
H10	0.0956	0.1351	0.5042	0.062*
C11	0.1574 (3)	0.2319 (7)	0.4169 (3)	0.0453 (15)
H11	0.2108	0.2012	0.4415	0.054*
C12	−0.0430 (3)	0.8604 (6)	−0.0863 (3)	0.0330 (12)
H12	−0.0934	0.8969	−0.1154	0.040*
C13	0.0317 (3)	0.9054 (6)	−0.1198 (3)	0.0317 (12)
C14	0.1123 (3)	0.8555 (7)	−0.0810 (3)	0.0350 (13)
C15	0.1849 (3)	0.8980 (7)	−0.1200 (3)	0.0465 (16)
H15	0.2376	0.8602	−0.0965	0.056*
C16	0.1787 (3)	0.9919 (7)	−0.1900 (3)	0.0432 (14)
H16	0.2274	1.0185	−0.2131	0.052*
C17	0.0997 (3)	1.0516 (7)	−0.2298 (3)	0.0384 (13)
C18	0.0255 (3)	1.0059 (7)	−0.1964 (3)	0.0350 (13)
C19	−0.0513 (3)	1.0648 (7)	−0.2389 (3)	0.0418 (14)
H19	−0.1014	1.0359	−0.2190	0.050*
C20	−0.0540 (3)	1.1632 (8)	−0.3086 (3)	0.0482 (14)
H20	−0.1057	1.1984	−0.3356	0.058*
C21	0.0196 (3)	1.2111 (7)	−0.3396 (3)	0.0511 (16)
H21	0.0175	1.2808	−0.3861	0.061*
C22	0.0946 (3)	1.1549 (7)	−0.3012 (3)	0.0448 (14)
H22	0.1438	1.1854	−0.3225	0.054*
C23	−0.1208 (3)	0.6324 (6)	0.0809 (3)	0.0307 (12)
C24	−0.1263 (3)	0.7353 (6)	0.0086 (3)	0.0320 (13)
C25	−0.2044 (3)	0.7904 (7)	−0.0266 (3)	0.0416 (14)
H25	−0.2085	0.8588	−0.0737	0.050*

C26	−0.2761 (3)	0.7462 (7)	0.0064 (3)	0.0475 (16)
H26	−0.3284	0.7839	−0.0181	0.057*
C27	−0.2700 (3)	0.6452 (7)	0.0765 (3)	0.0485 (15)
H27	−0.3184	0.6162	0.0996	0.058*
C28	−0.1933 (3)	0.5872 (7)	0.1123 (3)	0.0417 (14)
H28	−0.1904	0.5163	0.1584	0.050*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0257 (3)	0.0397 (4)	0.0389 (3)	−0.0006 (3)	0.0054 (2)	−0.0010 (4)
N1	0.024 (2)	0.032 (3)	0.035 (2)	−0.0032 (18)	0.0045 (18)	−0.001 (2)
N2	0.025 (2)	0.035 (3)	0.033 (2)	−0.0033 (18)	0.0060 (17)	0.0003 (19)
O1	0.0248 (18)	0.044 (3)	0.0412 (18)	−0.0052 (15)	0.0047 (15)	0.0049 (17)
O2	0.0286 (18)	0.057 (3)	0.0448 (19)	0.0001 (16)	0.0087 (15)	0.0111 (18)
C1	0.028 (3)	0.038 (4)	0.037 (3)	−0.004 (2)	0.011 (2)	−0.004 (3)
C2	0.026 (3)	0.034 (3)	0.036 (3)	0.002 (2)	0.005 (2)	−0.003 (2)
C3	0.028 (3)	0.031 (3)	0.040 (3)	−0.002 (2)	0.007 (2)	−0.008 (3)
C4	0.023 (3)	0.052 (4)	0.055 (3)	−0.001 (2)	0.008 (2)	0.005 (3)
C5	0.027 (3)	0.041 (4)	0.053 (3)	0.002 (3)	−0.002 (2)	−0.001 (3)
C6	0.033 (3)	0.034 (3)	0.041 (3)	0.000 (3)	0.005 (2)	−0.002 (3)
C7	0.034 (3)	0.027 (4)	0.039 (3)	−0.003 (2)	0.007 (2)	−0.007 (2)
C8	0.031 (3)	0.061 (4)	0.043 (3)	0.004 (3)	0.004 (2)	0.004 (3)
C9	0.044 (3)	0.071 (5)	0.052 (3)	0.007 (3)	0.011 (3)	0.009 (3)
C10	0.047 (3)	0.068 (5)	0.041 (3)	0.001 (3)	0.007 (3)	0.009 (3)
C11	0.040 (3)	0.048 (4)	0.047 (3)	0.006 (3)	0.001 (3)	0.007 (3)
C12	0.025 (3)	0.037 (4)	0.037 (3)	−0.001 (2)	0.003 (2)	−0.012 (3)
C13	0.029 (3)	0.036 (3)	0.030 (3)	−0.005 (2)	0.004 (2)	−0.006 (2)
C14	0.029 (3)	0.039 (4)	0.039 (3)	−0.003 (2)	0.007 (2)	−0.003 (3)
C15	0.027 (3)	0.067 (5)	0.048 (3)	0.004 (3)	0.015 (2)	0.000 (3)
C16	0.030 (3)	0.058 (4)	0.046 (3)	−0.002 (3)	0.021 (2)	−0.007 (3)
C17	0.039 (3)	0.040 (4)	0.037 (3)	0.000 (3)	0.012 (2)	−0.010 (3)
C18	0.038 (3)	0.036 (4)	0.032 (3)	−0.004 (3)	0.010 (2)	−0.013 (2)
C19	0.036 (3)	0.050 (4)	0.041 (3)	0.001 (3)	0.009 (2)	0.002 (3)
C20	0.047 (3)	0.052 (4)	0.045 (3)	0.006 (3)	0.003 (3)	0.000 (3)
C21	0.065 (4)	0.050 (5)	0.040 (3)	0.004 (3)	0.012 (3)	0.003 (3)
C22	0.050 (3)	0.048 (4)	0.041 (3)	−0.008 (3)	0.023 (2)	−0.006 (3)
C23	0.019 (2)	0.035 (4)	0.037 (3)	−0.003 (2)	0.003 (2)	−0.004 (2)
C24	0.024 (3)	0.037 (4)	0.036 (3)	0.000 (2)	0.005 (2)	−0.007 (2)
C25	0.029 (3)	0.056 (4)	0.039 (3)	0.001 (3)	0.000 (2)	0.010 (3)
C26	0.027 (3)	0.067 (5)	0.047 (3)	0.002 (3)	0.001 (2)	0.003 (3)
C27	0.027 (3)	0.068 (5)	0.052 (3)	−0.005 (3)	0.010 (2)	0.004 (3)
C28	0.026 (3)	0.051 (4)	0.048 (3)	−0.005 (2)	0.006 (2)	0.004 (3)

Geometric parameters (Å, °)

Cu1—O1	1.872 (3)	C12—C13	1.419 (6)
Cu1—O2	1.880 (3)	C12—H12	0.9300
Cu1—N1	1.913 (4)	C13—C14	1.421 (6)

Cu1—N2	1.919 (4)	C13—C18	1.467 (6)
N1—C1	1.306 (5)	C14—C15	1.431 (6)
N1—C23	1.428 (5)	C15—C16	1.350 (6)
N2—C12	1.300 (5)	C15—H15	0.9300
N2—C24	1.413 (5)	C16—C17	1.427 (6)
O1—C3	1.295 (5)	C16—H16	0.9300
O2—C14	1.289 (5)	C17—C22	1.410 (6)
C1—C2	1.422 (6)	C17—C18	1.413 (6)
C1—H1	0.9300	C18—C19	1.413 (6)
C2—C3	1.404 (6)	C19—C20	1.367 (6)
C2—C7	1.463 (6)	C19—H19	0.9300
C3—C4	1.426 (6)	C20—C21	1.390 (6)
C4—C5	1.346 (6)	C20—H20	0.9300
C4—H4	0.9300	C21—C22	1.358 (6)
C5—C6	1.412 (6)	C21—H21	0.9300
C5—H5	0.9300	C22—H22	0.9300
C6—C11	1.409 (6)	C23—C28	1.372 (6)
C6—C7	1.423 (6)	C23—C24	1.419 (6)
C7—C8	1.407 (6)	C24—C25	1.380 (5)
C8—C9	1.375 (6)	C25—C26	1.372 (6)
C8—H8	0.9300	C25—H25	0.9300
C9—C10	1.388 (6)	C26—C27	1.381 (6)
C9—H9	0.9300	C26—H26	0.9300
C10—C11	1.352 (6)	C27—C28	1.370 (6)
C10—H10	0.9300	C27—H27	0.9300
C11—H11	0.9300	C28—H28	0.9300
O1—Cu1—O2	87.91 (14)	C13—C12—H12	116.6
O1—Cu1—N1	93.25 (15)	C12—C13—C14	121.6 (4)
O2—Cu1—N1	178.02 (17)	C12—C13—C18	119.2 (4)
O1—Cu1—N2	178.18 (16)	C14—C13—C18	119.2 (4)
O2—Cu1—N2	93.75 (16)	O2—C14—C13	124.6 (4)
N1—Cu1—N2	85.10 (17)	O2—C14—C15	116.6 (4)
C1—N1—C23	121.2 (4)	C13—C14—C15	118.8 (4)
C1—N1—Cu1	125.5 (3)	C16—C15—C14	121.5 (5)
C23—N1—Cu1	113.0 (3)	C16—C15—H15	119.3
C12—N2—C24	122.0 (4)	C14—C15—H15	119.3
C12—N2—Cu1	124.8 (3)	C15—C16—C17	122.0 (5)
C24—N2—Cu1	113.1 (3)	C15—C16—H16	119.0
C3—O1—Cu1	128.3 (3)	C17—C16—H16	119.0
C14—O2—Cu1	128.1 (3)	C22—C17—C18	119.8 (5)
N1—C1—C2	126.1 (4)	C22—C17—C16	121.3 (5)
N1—C1—H1	117.0	C18—C17—C16	118.9 (5)
C2—C1—H1	117.0	C17—C18—C19	116.9 (5)
C3—C2—C1	121.3 (4)	C17—C18—C13	119.4 (4)
C3—C2—C7	119.4 (4)	C19—C18—C13	123.7 (4)
C1—C2—C7	119.2 (4)	C20—C19—C18	121.8 (5)
O1—C3—C2	125.3 (4)	C20—C19—H19	119.1
O1—C3—C4	116.1 (4)	C18—C19—H19	119.1
C2—C3—C4	118.6 (4)	C19—C20—C21	120.7 (5)

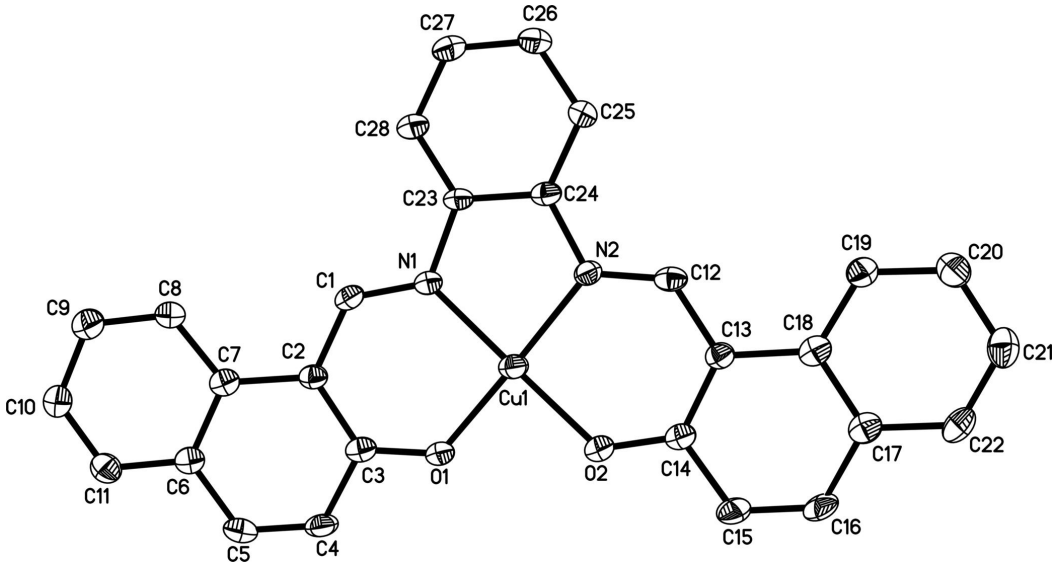
C5—C4—C3	122.4 (5)	C19—C20—H20	119.6
C5—C4—H4	118.8	C21—C20—H20	119.6
C3—C4—H4	118.8	C22—C21—C20	119.2 (5)
C4—C5—C6	121.4 (4)	C22—C21—H21	120.4
C4—C5—H5	119.3	C20—C21—H21	120.4
C6—C5—H5	119.3	C21—C22—C17	121.5 (5)
C11—C6—C5	119.8 (4)	C21—C22—H22	119.2
C11—C6—C7	121.1 (4)	C17—C22—H22	119.2
C5—C6—C7	119.1 (4)	C28—C23—C24	119.0 (4)
C8—C7—C6	116.2 (4)	C28—C23—N1	126.9 (4)
C8—C7—C2	124.7 (4)	C24—C23—N1	114.1 (4)
C6—C7—C2	119.1 (4)	C25—C24—N2	126.5 (4)
C9—C8—C7	122.1 (4)	C25—C24—C23	118.8 (4)
C9—C8—H8	119.0	N2—C24—C23	114.6 (4)
C7—C8—H8	119.0	C26—C25—C24	121.3 (5)
C8—C9—C10	119.9 (5)	C26—C25—H25	119.4
C8—C9—H9	120.0	C24—C25—H25	119.4
C10—C9—H9	120.0	C25—C26—C27	119.4 (5)
C11—C10—C9	121.0 (5)	C25—C26—H26	120.3
C11—C10—H10	119.5	C27—C26—H26	120.3
C9—C10—H10	119.5	C28—C27—C26	120.6 (5)
C10—C11—C6	119.8 (5)	C28—C27—H27	119.7
C10—C11—H11	120.1	C26—C27—H27	119.7
C6—C11—H11	120.1	C27—C28—C23	120.9 (5)
N2—C12—C13	126.8 (4)	C27—C28—H28	119.6
N2—C12—H12	116.6	C23—C28—H28	119.6

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O1^{i}	0.93	2.52	3.326 (6)	145

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

Fig. 1


C27
C26
C28
C25
C23
C24
N1
N2
C1
C12
C19
C20
C8
C9
C13
C18
C7
C2
C21
Cu1
C10
C17
C22
C3
O1
O2
C14
C11
C6
C15
C16
C5
C4