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# {$\mu_2$-1,4-Bis[2-(4-pyridyl)ethenyl]benzene-$\kappa^2N$:$N'$}bis[bis(acetylacetonato-$\kappa^2O,O'$)-copper(II)]

**Fang-Fang Jian,[a]* Jing Wang[b] and Jing Zhang[b]**

[a]Microscale Science Institute, Weifang University, Weifang 261061, People's Republic of China, and [b]New Materials and Function Coordination Chemistry Laboratory, Qingdao University of Science and Technology, Qingdao 266042, People's Republic of China
Correspondence e-mail: ffj2003@163169.com

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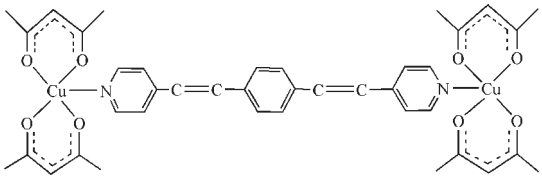
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.043; $wR$ factor = 0.113; data-to-parameter ratio = 14.3.

The asymmetric unit of the title compound, $[Cu_2(C_5H_7O_2)_4(C_{20}H_{16}N_2)]$, contains half of a centrosymmetric dinuclear molecule. In the molecule, each Cu center is coordinated by four O atoms from two acetylacetonate ligands and one N atom from the bridging linear 1,4-bis[2-(4-pyridyl)ethenyl]benzene ligand in a square-pyramidal geometry. In the crystal structure, weak intermolecular C—H···O hydrogen bonds link molecules into sheets parallel to the *bc* plane.

## Related literature

For coordination complexes with interesting topologies or properties, see: Ma *et al.* (2009); Liu *et al.* (2008). For long ligands, see: Banfi *et al.* (2002); Niu *et al.* (2001); Coe *et al.* (2006).



## Experimental

### Crystal data

$[Cu_2(C_5H_7O_2)_4(C_{20}H_{16}N_2)]$ $M_r$ = 807.85
Monoclinic, $P2_1/c$
$a$ = 7.9584 (16) Å
$b$ = 18.594 (4) Å
$c$ = 15.063 (4) Å
$\beta$ = 120.97 (2)°
$V$ = 1911.2 (8) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 1.17 mm$^{-1}$
$T$ = 293 K
0.25 × 0.21 × 0.20 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2000)
$T_{min}$ = 0.759, $T_{max}$ = 0.800
7784 measured reflections
3352 independent reflections
2807 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.022

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.113
$S$ = 0.99
3352 reflections
235 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.41 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.19 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C14—H14$A$···O2$^{i}$ | 0.93 | 2.45 | 3.371 (4) | 173 |
| C16—H16$A$···O1$^{ii}$ | 0.93 | 2.52 | 3.333 (4) | 147 |
| C16—H16$A$···O3$^{ii}$ | 0.93 | 2.58 | 3.315 (4) | 136 |

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

This work was supported financially by the Doctoral Fund of Shandaong Province (No. 2007BS04046).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2655).

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# supporting information

*Acta Cryst.* (2009). E**65**, m1630 [doi:10.1107/S1600536809048582]

## {$\mu_2$-1,4-Bis[2-(4-pyridyl)ethenyl]benzene-$\kappa^2N$:$N'$}bis[bis(acetylacetonato-$\kappa^2O,O'$)copper(II)]

**Fang-Fang Jian, Jing Wang and Jing Zhang**

### S1. Comment

Metal ions and organic ligands are considered as the most important factors for designing the coordination networks (Ma *et al.*, 2009). Up to now, it is still a challenge to predict the exact structure and understand the roles of both factors in crystal engineering. The flexible bridging ligands can afford different conformation with interesting topologies or properties (Liu *et al.*, 2008). Among the others, long bis(pyridyl) ligands are used to construct the connectivity and geometry with different coordination sites metal ions, and often lead to interesting structural motifs (Ma *et al.*, 2009). A large number of examples of particularly long ligands - 1,4-phenylenebis(4-pyridylmethanone), bis(4-pyridyl)-terephthalate (Banfi *et al.*, 2002), *N*,*N*′-bis(4-pyridylmethyl)piperazine (Niu *et al.*, 2001), *N*-phenyl-1,4-bis(*E*-2-(4-pyridyl)ethenyl)benzene (Coe *et al.*, 2006), have been adopted for the self-assembly of coordination polymers, such as one-dimensional coordination chains, double helices, two dimensional layered structures, interpenetrated ladders, interpenetrated frameworks and so on (Banfi *et al.*, 2002). Herein, we present the shoulder-pole coordination compound based on 1,4-bis(2-(4-pyridyl)ethenyl)benzole (bpyph) ligand, and describe its crystal structure.

In the title structure (Fig. 1),each Cu center is coordinated by four O atoms and one N atom from the bpyph ligand in a distorted pyramidal geometry. The linear bpyph ligand links two acetylacetonate copper(II) by Cu—N bonds, displaying the shoulder-pole model. In the crystal structure, weak intermolecular C—H···O hydrogen bonds (Table 1) link molecules into sheets parallel to *bc* plane.

### S2. Experimental

1,4-Bis(2-(4-pyridyl)ethenyl)benzene (2.84 g, 0.01 mol) and acetylacetonate copper(II) (5.23 g, 0.02 mol) in 2:1 molar ratio was dissolved in ethanol solution (40 ml) and refluxed for 2 h. After cooling and filtering, the blue block crystals were collected after 4 days (yield 42.35%).

### S3. Refinement

All H atoms were positioned geometrically (C—H 0.93–0.96 Å) and allowed to ride on their parent atoms, with $U_{iso}$(H) = 1.2$U_{eq}$ of the parent atom.

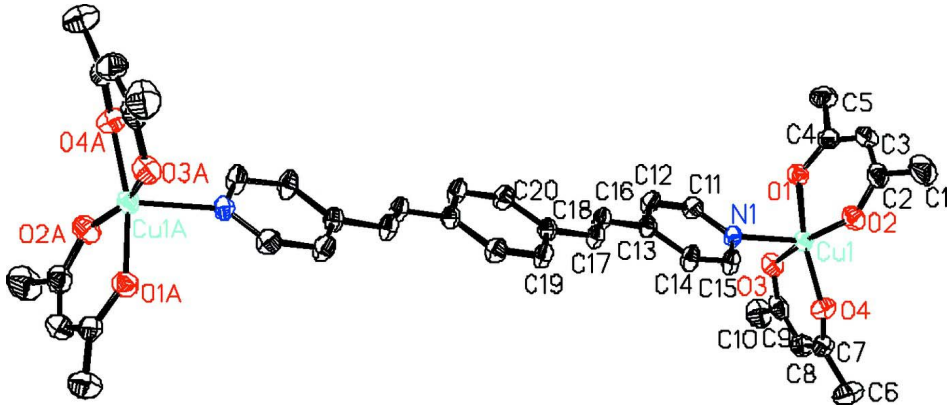


**Figure 1**

The molecular structure of the title compound with the atom-labeling scheme [symmetry code: (A) 1-x, -y, 1-z]. H atoms omited for clarity. Displacement ellipsoids are drawn at the 30% probability level.

**{$\mu_2$-1,4-Bis[2-(4-pyridyl)ethenyl]benzene- $\kappa^2N$:$N'$}bis[bis(acetylacetonato- $\kappa^2O,O'$)copper(II)]**

*Crystal data*

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Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 7.9584$ (16) Å
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$c = 15.063$ (4) Å
$\beta = 120.97$ (2)°
$V = 1911.2$ (8) Å$^3$
$Z = 2$
$F(000) = 840$
$D_x = 1.404$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1253 reflections
$\theta = 1.9$–25.0°
$\mu = 1.17$ mm$^{-1}$
$T = 293$ K
Block, blue
0.25 × 0.21 × 0.20 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2000)
$T_{min} = 0.759$, $T_{max} = 0.800$
7784 measured reflections
3352 independent reflections
2807 reflections with $I > 2\sigma(I)$
$R_{int} = 0.022$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.9°$
$h = -9\rightarrow5$
$k = -22\rightarrow20$
$l = -17\rightarrow17$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.113$
$S = 0.99$
3352 reflections
235 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
$w = 1/[\sigma^2(F_o^2) + (0.0573P)^2 + 1.3432P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.41$ e Å$^{-3}$
$\Delta\rho_{min} = -0.19$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cu1 | 0.51253 (5) | −0.173135 (19) | −0.13916 (3) | 0.04299 (16) |
| O1 | 0.3204 (3) | −0.25040 (12) | −0.18542 (17) | 0.0531 (6) |
| O2 | 0.3110 (3) | −0.10340 (12) | −0.22282 (18) | 0.0586 (6) |
| O3 | 0.7113 (3) | −0.24740 (12) | −0.09329 (17) | 0.0564 (6) |
| O4 | 0.6960 (3) | −0.09862 (12) | −0.12417 (19) | 0.0604 (6) |
| N1 | 0.5307 (4) | −0.15375 (13) | 0.01154 (18) | 0.0414 (6) |
| C1 | 0.0211 (6) | −0.0532 (3) | −0.3578 (4) | 0.0995 (16) |
| H1A | 0.1015 | −0.0110 | −0.3323 | 0.149* |
| H1B | −0.0934 | −0.0470 | −0.3527 | 0.149* |
| H1C | −0.0177 | −0.0609 | −0.4288 | 0.149* |
| C2 | 0.1362 (5) | −0.1177 (2) | −0.2939 (3) | 0.0629 (9) |
| C3 | 0.0540 (5) | −0.1850 (2) | −0.3146 (3) | 0.0691 (11) |
| H3A | −0.0755 | −0.1890 | −0.3684 | 0.083* |
| C4 | 0.1463 (5) | −0.2471 (2) | −0.2628 (3) | 0.0579 (9) |
| C5 | 0.0410 (7) | −0.3181 (2) | −0.2979 (4) | 0.0868 (14) |
| H5A | 0.1251 | −0.3558 | −0.2540 | 0.130* |
| H5B | 0.0066 | −0.3271 | −0.3681 | 0.130* |
| H5C | −0.0757 | −0.3165 | −0.2942 | 0.130* |
| C6 | 0.9651 (7) | −0.0436 (3) | −0.1201 (4) | 0.1045 (17) |
| H6A | 0.8839 | −0.0022 | −0.1323 | 0.157* |
| H6B | 0.9885 | −0.0490 | −0.1763 | 0.157* |
| H6C | 1.0878 | −0.0374 | −0.0565 | 0.157* |
| C7 | 0.8632 (6) | −0.1098 (2) | −0.1128 (3) | 0.0648 (10) |
| C8 | 0.9518 (6) | −0.1755 (2) | −0.0957 (3) | 0.0747 (12) |
| H8A | 1.0737 | −0.1769 | −0.0901 | 0.090* |
| C9 | 0.8778 (5) | −0.2392 (2) | −0.0861 (3) | 0.0623 (10) |
| C10 | 0.9943 (7) | −0.3073 (3) | −0.0657 (4) | 0.0896 (14) |
| H10A | 0.9217 | −0.3470 | −0.0616 | 0.134* |
| H10B | 1.1167 | −0.3029 | −0.0015 | 0.134* |
| H10C | 1.0187 | −0.3154 | −0.1210 | 0.134* |
| C11 | 0.4967 (5) | −0.20205 (18) | 0.0647 (2) | 0.0505 (8) |
| H11A | 0.4738 | −0.2492 | 0.0409 | 0.061* |
| C12 | 0.4930 (5) | −0.18686 (17) | 0.1532 (2) | 0.0519 (8) |
| H12A | 0.4707 | −0.2235 | 0.1879 | 0.062* |
| C13 | 0.5224 (4) | −0.11714 (16) | 0.1905 (2) | 0.0434 (7) |

| | | | | |
|---|---|---|---|---|
| C14 | 0.5614 (5) | −0.06650 (17) | 0.1356 (2) | 0.0514 (8) |
| H14A | 0.5842 | −0.0188 | 0.1573 | 0.062* |
| C15 | 0.5661 (5) | −0.08703 (17) | 0.0498 (2) | 0.0513 (8) |
| H15A | 0.5959 | −0.0522 | 0.0157 | 0.062* |
| C16 | 0.5141 (5) | −0.10005 (17) | 0.2825 (2) | 0.0488 (8) |
| H16A | 0.5061 | −0.1388 | 0.3192 | 0.059* |
| C17 | 0.5167 (5) | −0.03530 (16) | 0.3193 (2) | 0.0451 (7) |
| H17A | 0.5261 | 0.0034 | 0.2830 | 0.054* |
| C18 | 0.5065 (4) | −0.01843 (16) | 0.4102 (2) | 0.0420 (7) |
| C19 | 0.5343 (5) | 0.05182 (16) | 0.4469 (2) | 0.0501 (8) |
| H19A | 0.5577 | 0.0877 | 0.4115 | 0.060* |
| C20 | 0.4717 (5) | −0.07005 (17) | 0.4662 (2) | 0.0505 (8) |
| H20A | 0.4522 | −0.1177 | 0.4444 | 0.061* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cu1 | 0.0456 (2) | 0.0468 (2) | 0.0388 (2) | 0.00112 (16) | 0.02331 (18) | −0.00511 (16) |
| O1 | 0.0523 (14) | 0.0536 (13) | 0.0514 (13) | −0.0059 (10) | 0.0252 (11) | −0.0089 (10) |
| O2 | 0.0541 (15) | 0.0537 (14) | 0.0549 (14) | 0.0064 (11) | 0.0186 (12) | −0.0004 (11) |
| O3 | 0.0531 (14) | 0.0571 (14) | 0.0565 (14) | 0.0087 (11) | 0.0263 (12) | −0.0045 (11) |
| O4 | 0.0600 (15) | 0.0584 (14) | 0.0720 (16) | −0.0050 (11) | 0.0405 (13) | −0.0016 (12) |
| N1 | 0.0477 (15) | 0.0439 (14) | 0.0347 (13) | 0.0026 (11) | 0.0226 (11) | −0.0037 (10) |
| C1 | 0.073 (3) | 0.101 (4) | 0.094 (4) | 0.027 (3) | 0.021 (3) | 0.024 (3) |
| C2 | 0.054 (2) | 0.080 (3) | 0.052 (2) | 0.0147 (19) | 0.0260 (18) | 0.0080 (18) |
| C3 | 0.045 (2) | 0.093 (3) | 0.055 (2) | −0.006 (2) | 0.0155 (17) | 0.003 (2) |
| C4 | 0.055 (2) | 0.077 (2) | 0.049 (2) | −0.0143 (18) | 0.0314 (18) | −0.0138 (18) |
| C5 | 0.076 (3) | 0.094 (3) | 0.084 (3) | −0.035 (2) | 0.037 (3) | −0.021 (2) |
| C6 | 0.088 (3) | 0.118 (4) | 0.122 (4) | −0.030 (3) | 0.065 (3) | 0.000 (3) |
| C7 | 0.059 (2) | 0.089 (3) | 0.053 (2) | −0.012 (2) | 0.0331 (19) | −0.0033 (19) |
| C8 | 0.050 (2) | 0.103 (3) | 0.078 (3) | 0.007 (2) | 0.038 (2) | 0.008 (2) |
| C9 | 0.053 (2) | 0.089 (3) | 0.0406 (18) | 0.019 (2) | 0.0211 (17) | −0.0028 (18) |
| C10 | 0.077 (3) | 0.110 (4) | 0.084 (3) | 0.037 (3) | 0.043 (3) | 0.008 (3) |
| C11 | 0.064 (2) | 0.0442 (17) | 0.0515 (19) | −0.0086 (15) | 0.0354 (17) | −0.0137 (15) |
| C12 | 0.076 (2) | 0.0423 (17) | 0.052 (2) | −0.0084 (15) | 0.0434 (19) | −0.0021 (14) |
| C13 | 0.0547 (19) | 0.0422 (16) | 0.0375 (16) | 0.0041 (14) | 0.0269 (14) | −0.0002 (13) |
| C14 | 0.083 (2) | 0.0383 (17) | 0.0457 (18) | 0.0030 (16) | 0.0419 (18) | −0.0020 (13) |
| C15 | 0.076 (2) | 0.0444 (18) | 0.0431 (17) | 0.0049 (16) | 0.0371 (17) | 0.0047 (14) |
| C16 | 0.071 (2) | 0.0450 (18) | 0.0416 (17) | 0.0018 (15) | 0.0368 (16) | 0.0023 (13) |
| C17 | 0.061 (2) | 0.0444 (17) | 0.0392 (16) | 0.0014 (14) | 0.0329 (15) | 0.0028 (13) |
| C18 | 0.0495 (18) | 0.0436 (16) | 0.0356 (15) | 0.0021 (13) | 0.0239 (14) | −0.0014 (13) |
| C19 | 0.075 (2) | 0.0424 (17) | 0.0457 (18) | −0.0034 (15) | 0.0401 (17) | 0.0014 (13) |
| C20 | 0.074 (2) | 0.0399 (17) | 0.0471 (18) | −0.0049 (15) | 0.0379 (17) | −0.0075 (14) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cu1—O2 | 1.939 (2) | C7—C8 | 1.367 (5) |
| Cu1—O4 | 1.940 (2) | C8—C9 | 1.363 (6) |

| | | | |
|---|---|---|---|
| Cu1—O3 | 1.940 (2) | C8—H8A | 0.9300 |
| Cu1—O1 | 1.947 (2) | C9—C10 | 1.504 (5) |
| Cu1—N1 | 2.228 (2) | C10—H10A | 0.9600 |
| O1—C4 | 1.273 (4) | C10—H10B | 0.9600 |
| O2—C2 | 1.273 (4) | C10—H10C | 0.9600 |
| O3—C9 | 1.282 (4) | C11—C12 | 1.378 (4) |
| O4—C7 | 1.269 (4) | C11—H11A | 0.9300 |
| N1—C11 | 1.320 (4) | C12—C13 | 1.384 (4) |
| N1—C15 | 1.335 (4) | C12—H12A | 0.9300 |
| C1—C2 | 1.515 (5) | C13—C14 | 1.389 (4) |
| C1—H1A | 0.9600 | C13—C16 | 1.456 (4) |
| C1—H1B | 0.9600 | C14—C15 | 1.368 (4) |
| C1—H1C | 0.9600 | C14—H14A | 0.9300 |
| C2—C3 | 1.371 (5) | C15—H15A | 0.9300 |
| C3—C4 | 1.376 (5) | C16—C17 | 1.321 (4) |
| C3—H3A | 0.9300 | C16—H16A | 0.9300 |
| C4—C5 | 1.505 (5) | C17—C18 | 1.448 (4) |
| C5—H5A | 0.9600 | C17—H17A | 0.9300 |
| C5—H5B | 0.9600 | C18—C19 | 1.391 (4) |
| C5—H5C | 0.9600 | C18—C20 | 1.397 (4) |
| C6—C7 | 1.511 (6) | C19—C20$^{i}$ | 1.376 (4) |
| C6—H6A | 0.9600 | C19—H19A | 0.9300 |
| C6—H6B | 0.9600 | C20—C19$^{i}$ | 1.376 (4) |
| C6—H6C | 0.9600 | C20—H20A | 0.9300 |

| | | | |
|---|---|---|---|
| O2—Cu1—O4 | 85.37 (10) | O4—C7—C6 | 114.9 (4) |
| O2—Cu1—O3 | 163.25 (10) | C8—C7—C6 | 119.9 (4) |
| O4—Cu1—O3 | 92.29 (11) | C9—C8—C7 | 125.9 (4) |
| O2—Cu1—O1 | 91.51 (10) | C9—C8—H8A | 117.0 |
| O4—Cu1—O1 | 166.93 (10) | C7—C8—H8A | 117.0 |
| O3—Cu1—O1 | 87.05 (10) | O3—C9—C8 | 125.4 (3) |
| O2—Cu1—N1 | 98.77 (10) | O3—C9—C10 | 114.7 (4) |
| O4—Cu1—N1 | 96.62 (10) | C8—C9—C10 | 119.9 (4) |
| O3—Cu1—N1 | 97.98 (9) | C9—C10—H10A | 109.5 |
| O1—Cu1—N1 | 96.40 (9) | C9—C10—H10B | 109.5 |
| C4—O1—Cu1 | 125.2 (2) | H10A—C10—H10B | 109.5 |
| C2—O2—Cu1 | 125.9 (2) | C9—C10—H10C | 109.5 |
| C9—O3—Cu1 | 124.3 (2) | H10A—C10—H10C | 109.5 |
| C7—O4—Cu1 | 124.9 (2) | H10B—C10—H10C | 109.5 |
| C11—N1—C15 | 115.7 (3) | N1—C11—C12 | 124.1 (3) |
| C11—N1—Cu1 | 125.5 (2) | N1—C11—H11A | 118.0 |
| C15—N1—Cu1 | 118.6 (2) | C12—C11—H11A | 118.0 |
| C2—C1—H1A | 109.5 | C11—C12—C13 | 120.1 (3) |
| C2—C1—H1B | 109.5 | C11—C12—H12A | 120.0 |
| H1A—C1—H1B | 109.5 | C13—C12—H12A | 120.0 |
| C2—C1—H1C | 109.5 | C12—C13—C14 | 115.9 (3) |
| H1A—C1—H1C | 109.5 | C12—C13—C16 | 120.6 (3) |
| H1B—C1—H1C | 109.5 | C14—C13—C16 | 123.5 (3) |

| | | | |
|---|---|---|---|
| O2—C2—C3 | 124.7 (3) | C15—C14—C13 | 119.8 (3) |
| O2—C2—C1 | 114.2 (4) | C15—C14—H14A | 120.1 |
| C3—C2—C1 | 121.1 (4) | C13—C14—H14A | 120.1 |
| C2—C3—C4 | 125.7 (3) | N1—C15—C14 | 124.4 (3) |
| C2—C3—H3A | 117.1 | N1—C15—H15A | 117.8 |
| C4—C3—H3A | 117.1 | C14—C15—H15A | 117.8 |
| O1—C4—C3 | 124.8 (3) | C17—C16—C13 | 126.8 (3) |
| O1—C4—C5 | 115.3 (3) | C17—C16—H16A | 116.6 |
| C3—C4—C5 | 119.9 (3) | C13—C16—H16A | 116.6 |
| C4—C5—H5A | 109.5 | C16—C17—C18 | 126.7 (3) |
| C4—C5—H5B | 109.5 | C16—C17—H17A | 116.6 |
| H5A—C5—H5B | 109.5 | C18—C17—H17A | 116.6 |
| C4—C5—H5C | 109.5 | C19—C18—C20 | 116.5 (3) |
| H5A—C5—H5C | 109.5 | C19—C18—C17 | 120.3 (3) |
| H5B—C5—H5C | 109.5 | C20—C18—C17 | 123.2 (3) |
| C7—C6—H6A | 109.5 | C20$^{i}$—C19—C18 | 122.2 (3) |
| C7—C6—H6B | 109.5 | C20$^{i}$—C19—H19A | 118.9 |
| H6A—C6—H6B | 109.5 | C18—C19—H19A | 118.9 |
| C7—C6—H6C | 109.5 | C19$^{i}$—C20—C18 | 121.3 (3) |
| H6A—C6—H6C | 109.5 | C19$^{i}$—C20—H20A | 119.3 |
| H6B—C6—H6C | 109.5 | C18—C20—H20A | 119.3 |
| O4—C7—C8 | 125.2 (4) | | |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C14—H14*A*···O2$^{ii}$ | 0.93 | 2.45 | 3.371 (4) | 173 |
| C16—H16*A*···O1$^{iii}$ | 0.93 | 2.52 | 3.333 (4) | 147 |
| C16—H16*A*···O3$^{iii}$ | 0.93 | 2.58 | 3.315 (4) | 136 |

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