

Bis[2,4-dichloro-6-(piperidin-1-ylmethyl)-phenolato- $\kappa^2 N,O$]copper(II)

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Key indicators

Single-crystal X-ray study

$T = 298\text{ K}$

Mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$

R factor = 0.034

wR factor = 0.098

Data-to-parameter ratio = 13.3

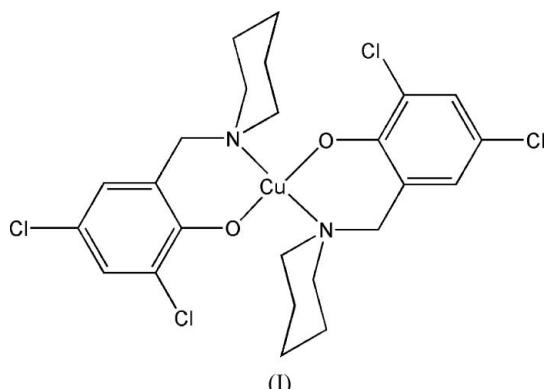
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

In the title compound, $[\text{Cu}(\text{C}_{12}\text{H}_{14}\text{Cl}_2\text{NO})_2]$, the Cu^{II} atom is four-coordinated in a distorted square-planar geometry by two N atoms and two O atoms from two 2,4-dichloro-6-(piperidin-1-ylmethyl)phenolate ligands. The dihedral angle between the N/Cu/O coordination planes is $16.53(9)^\circ$.

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Comment

Piperidine compounds can act as complexing reagents with metallic ions, but few metal complexes with piperidine derivatives have been reported (Näther & Beck, 2004). Recently, we determined the crystal structure of 2,4-dichloro-6-(piperidin-1-ylmethyl)phenol (HCl_2bpipe) in which intermolecular $\text{C}\cdots\text{C}$ and $\text{Cl}\cdots\text{Cl}$ contacts were observed (Kubono *et al.*, 2005). The present paper describes the crystal structure of the Cu^{II} complex with HCl_2bpipe , (I).



The molecular structure of (I) is shown in Fig. 1. The Cu^{II} atom is four-coordinated by two amine N atoms and two phenolate O atoms derived from two bidentate 2,4-dichloro-6-(piperidin-1-ylmethyl)phenolate ligands. The geometry of the coordination is distorted square-planar. The dihedral angle between the N/Cu/O coordination planes is $16.53(9)^\circ$. The $\text{Cu}-\text{O}$ and $\text{Cu}-\text{N}$ bond lengths are comparable to those of other aminophenol Cu^{II} complexes (You, 2005; Chen *et al.*, 2005). In the crystal structure, no significant intermolecular interactions are observed.

Experimental

HCl_2bpipe (0.104 g, 0.4 mmol) was dissolved in 20 ml of hot chloroform and 30 ml of a methanol solution of copper(II) acetate monohydrate (0.040 g, 0.2 mmol) were then added to this solution. The mixture was stirred for 20 min at 340 K. After a few days at room temperature, brown crystals of (I) were obtained. Yield 86.9%; m.p. 465.0–465.7 K. Analysis calculated for $\text{C}_{24}\text{H}_{28}\text{Cl}_4\text{CuN}_2\text{O}_2$: C 49.54, H 4.85, N 4.81%; found: C 49.45, H 4.89, N 4.79%.

Crystal data $[\text{Cu}(\text{C}_{12}\text{H}_{14}\text{Cl}_2\text{NO})_2]$ $M_r = 581.83$ Monoclinic, $P2_1/n$ $a = 12.602 (6) \text{ \AA}$ $b = 18.049 (16) \text{ \AA}$ $c = 11.123 (4) \text{ \AA}$ $\beta = 95.07 (4)^\circ$ $V = 2520 (3) \text{ \AA}^3$ $Z = 4$ $D_x = 1.534 \text{ Mg m}^{-3}$ Mo $K\alpha$ radiation $\mu = 1.32 \text{ mm}^{-1}$ $T = 298.1 \text{ K}$

Prism, brown

 $0.23 \times 0.20 \times 0.18 \text{ mm}$ **Data collection**Rigaku AFC7R diffractometer
 ω - 2θ scansAbsorption correction: ψ scan
(North *et al.*, 1968) $T_{\min} = 0.733$, $T_{\max} = 0.789$

6951 measured reflections

5790 independent reflections

4342 reflections with $F^2 > 2\sigma(F^2)$ $R_{\text{int}} = 0.021$ $\theta_{\max} = 27.5^\circ$

3 standard reflections

every 150 reflections

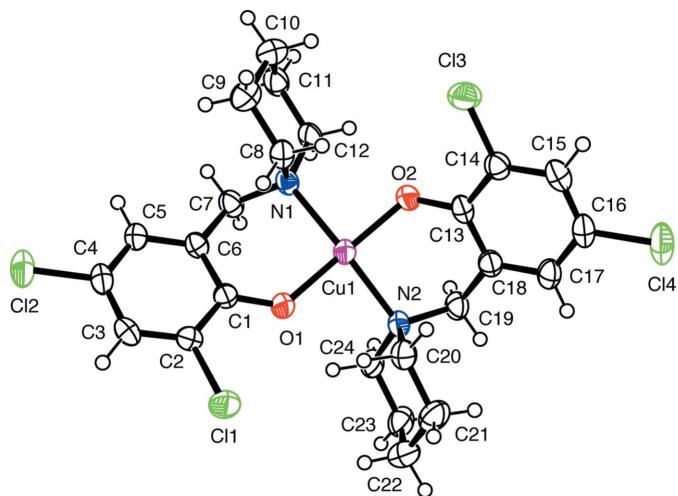
intensity decay: 0.2%

RefinementRefinement on F^2 $R[F^2 > 2\sigma(F^2)] = 0.034$ $wR(F^2) = 0.098$ $S = 1.00$

4342 reflections

326 parameters

H-atom parameters constrained

 $w = 1/[0.0011F_o^2 + \sigma(F_o^2)]/(4F_o^2)$ $(\Delta/\sigma)_{\max} < 0.001$ $\Delta\rho_{\max} = 0.42 \text{ e \AA}^{-3}$ $\Delta\rho_{\min} = -0.48 \text{ e \AA}^{-3}$ **Figure 1**

The molecular structure of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented by circles of arbitrary size.

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Table 1Selected geometric parameters (\AA , $^\circ$).

Cu1—O1	1.894 (2)	Cu1—N1	2.074 (2)
Cu1—O2	1.895 (2)	Cu1—N2	2.072 (2)
O1—Cu1—O2	166.02 (9)	O2—Cu1—N1	88.97 (9)
O1—Cu1—N1	92.60 (9)	O2—Cu1—N2	93.76 (9)
O1—Cu1—N2	86.99 (9)	N1—Cu1—N2	170.32 (9)

All H atoms were placed at idealized positions and refined as riding atoms, with C—H distance of 0.95 \AA and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: *WinAFC* (Rigaku/MSC, 2004); cell refinement: *WinAFC*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *CrystalStructure*.

References

- Altomare, A., Casciaro, G., Giacovazzo, C., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435.
- Betteridge, P. W., Carruthers, J. R., Cooper, R. I., Prout, K. & Watkin, D. J. (2003). *J. Appl. Cryst.* **36**, 1487.
- Chen, L., Zhou, H., Pan, Z.-Q., Hu, X.-L. & Liu, B. (2005). *Acta Cryst. E61*, m1467–m1469.
- Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
- Kubono, K., Oshima, S., Hirayama, N. & Yokoi, K. (2005). *Acta Cryst. E61*, o3706–o3708.
- Näther, C. & Beck, A. (2004). *Acta Cryst. E60*, m1008–m1009.
- North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst. A24*, 351–359.
- Rigaku/MSC (2004). *WinAFC* and *CrystalStructure*. Version 3.7.0. Rigaku/MSC, The Woodlands, Texas, USA.
- You, Z.-L. (2005). *Acta Cryst. C61*, m406–m408.

supporting information

Acta Cryst. (2006). E62, m2858–m2859 [https://doi.org/10.1107/S1600536806040207]

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(I)

Crystal data



$M_r = 581.83$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 12.602 (6)$ Å

$b = 18.049 (16)$ Å

$c = 11.123 (4)$ Å

$\beta = 95.07 (4)^\circ$

$V = 2520 (3)$ Å³

$Z = 4$

$F(000) = 1196.00$

$D_x = 1.534$ Mg m⁻³

Melting point = 465.0–465.7 K

Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å

Cell parameters from 25 reflections

$\theta = 15.2\text{--}17.5^\circ$

$\mu = 1.32$ mm⁻¹

$T = 298$ K

Prism, brown

0.23 × 0.20 × 0.18 mm

Data collection

Rigaku AFC7R

diffractometer

ω -2θ scans

Absorption correction: ψ scan

(North *et al.*, 1968)

$T_{\min} = 0.733$, $T_{\max} = 0.789$

6951 measured reflections

5790 independent reflections

4342 reflections with $F^2 > 2.0\sigma(F^2)$

$R_{\text{int}} = 0.021$

$\theta_{\max} = 27.5^\circ$

$h = -9 \rightarrow 16$

$k = 0 \rightarrow 23$

$l = -14 \rightarrow 14$

3 standard reflections every 150 reflections

intensity decay: 0.2%

Refinement

Refinement on F^2

$R[F^2 > 2\sigma(F^2)] = 0.034$

$wR(F^2) = 0.098$

$S = 1.00$

4342 reflections

326 parameters

H-atom parameters constrained

$w = 1/[0.0011F_o^2 + 1.0000\sigma(F_o^2)]/(4F_o^2)$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.42$ e Å⁻³

$\Delta\rho_{\min} = -0.48$ e Å⁻³

Special details

Geometry. ENTER SPECIAL DETAILS OF THE MOLECULAR GEOMETRY

Refinement. Refinement using reflections with $F^2 > 2.0\sigma(F^2)$. The weighted R -factor (wR) and goodness of fit (S) are based on F^2 . R -factor (gt) are based on F . The threshold expression of $F^2 > 2.0\sigma(F^2)$ is used only for calculating R -factor (gt).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.09898 (3)	0.16797 (2)	0.98617 (3)	0.03156 (10)

Cl1	-0.21438 (6)	0.02624 (5)	0.94133 (8)	0.0479 (2)
Cl2	-0.32469 (8)	0.10956 (6)	1.37819 (9)	0.0633 (3)
Cl3	0.44897 (6)	0.11495 (5)	1.11187 (8)	0.0519 (2)
Cl4	0.53078 (8)	0.04436 (6)	0.65810 (10)	0.0631 (3)
O1	-0.04435 (17)	0.13657 (12)	0.98665 (18)	0.0412 (6)
O2	0.24947 (17)	0.17471 (12)	0.99362 (19)	0.0378 (6)
N1	0.10586 (19)	0.20210 (12)	1.1647 (2)	0.0324 (7)
N2	0.0824 (2)	0.15166 (12)	0.8011 (2)	0.0311 (6)
C1	-0.1049 (2)	0.13014 (17)	1.0771 (2)	0.0313 (8)
C2	-0.1925 (2)	0.08186 (17)	1.0695 (2)	0.0315 (8)
C3	-0.2603 (2)	0.07486 (17)	1.1595 (2)	0.0344 (8)
C4	-0.2395 (2)	0.11723 (19)	1.2625 (2)	0.0392 (9)
C5	-0.1546 (2)	0.16478 (18)	1.2755 (2)	0.0361 (8)
C6	-0.0879 (2)	0.17236 (16)	1.1831 (2)	0.0314 (7)
C7	-0.0013 (2)	0.22924 (18)	1.1913 (2)	0.0373 (9)
C8	0.1427 (2)	0.13497 (19)	1.2362 (2)	0.0367 (8)
C9	0.1651 (3)	0.1487 (2)	1.3708 (2)	0.0551 (11)
C10	0.2454 (3)	0.2118 (2)	1.3941 (3)	0.0663 (14)
C11	0.2079 (2)	0.2799 (2)	1.3252 (3)	0.0534 (11)
C12	0.1855 (2)	0.26303 (18)	1.1917 (2)	0.0414 (9)
C13	0.3101 (2)	0.14317 (17)	0.9178 (2)	0.0333 (8)
C14	0.4093 (2)	0.11336 (17)	0.9580 (2)	0.0366 (8)
C15	0.4773 (2)	0.08212 (18)	0.8799 (3)	0.0398 (9)
C16	0.4450 (2)	0.08029 (18)	0.7583 (3)	0.0409 (9)
C17	0.3474 (2)	0.10828 (18)	0.7153 (2)	0.0386 (9)
C18	0.2805 (2)	0.13997 (18)	0.7926 (2)	0.0351 (8)
C19	0.1791 (2)	0.17771 (18)	0.7455 (2)	0.0376 (9)
C20	0.0642 (2)	0.07041 (17)	0.7813 (2)	0.0383 (9)
C21	0.0314 (3)	0.0498 (2)	0.6508 (3)	0.0527 (11)
C22	-0.0647 (3)	0.0944 (2)	0.6002 (3)	0.0646 (13)
C23	-0.0444 (2)	0.1765 (2)	0.6166 (2)	0.0518 (11)
C24	-0.0117 (2)	0.19462 (19)	0.7477 (2)	0.0380 (9)
H1	-0.3197	0.0423	1.1509	0.041*
H2	-0.1418	0.1931	1.3473	0.044*
H3	0.0047	0.2486	1.2710	0.045*
H4	-0.0217	0.2677	1.1357	0.045*
H5	0.0890	0.0981	1.2239	0.044*
H6	0.2064	0.1177	1.2060	0.044*
H7	0.1005	0.1619	1.4034	0.066*
H8	0.1930	0.1049	1.4091	0.066*
H9	0.2549	0.2226	1.4780	0.079*
H10	0.3116	0.1970	1.3670	0.079*
H11	0.1437	0.2963	1.3554	0.065*
H12	0.2602	0.3178	1.3363	0.065*
H13	0.2508	0.2491	1.1612	0.050*
H14	0.1587	0.3064	1.1512	0.050*
H15	0.5446	0.0628	0.9096	0.048*
H16	0.3261	0.1058	0.6313	0.047*

H17	0.1691	0.1703	0.6607	0.046*
H18	0.1870	0.2291	0.7622	0.046*
H19	0.1279	0.0448	0.8076	0.046*
H20	0.0088	0.0554	0.8285	0.046*
H21	0.0890	0.0606	0.6041	0.064*
H22	0.0156	-0.0016	0.6458	0.064*
H23	-0.0804	0.0833	0.5170	0.077*
H24	-0.1238	0.0813	0.6432	0.077*
H25	0.0121	0.1899	0.5697	0.062*
H26	-0.1066	0.2036	0.5897	0.062*
H27	-0.0705	0.1845	0.7930	0.046*
H28	0.0058	0.2457	0.7541	0.046*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0296 (2)	0.0348 (2)	0.0310 (2)	-0.00147 (18)	0.00635 (14)	-0.00136 (17)
Cl1	0.0498 (5)	0.0483 (5)	0.0455 (4)	-0.0127 (4)	0.0036 (4)	-0.0119 (4)
Cl2	0.0532 (5)	0.0868 (7)	0.0543 (5)	-0.0147 (5)	0.0282 (4)	-0.0040 (5)
Cl3	0.0461 (5)	0.0592 (6)	0.0482 (5)	0.0103 (4)	-0.0077 (4)	-0.0089 (4)
Cl4	0.0527 (6)	0.0683 (6)	0.0735 (6)	0.0066 (5)	0.0340 (5)	-0.0113 (5)
O1	0.0349 (12)	0.0560 (14)	0.0336 (11)	-0.0137 (11)	0.0089 (9)	-0.0077 (10)
O2	0.0277 (11)	0.0471 (13)	0.0387 (11)	0.0031 (10)	0.0036 (9)	-0.0100 (10)
N1	0.0284 (14)	0.0297 (13)	0.0399 (14)	-0.0019 (11)	0.0078 (11)	-0.0065 (11)
N2	0.0281 (13)	0.0336 (14)	0.0324 (13)	0.0040 (10)	0.0075 (10)	0.0029 (10)
C1	0.0294 (16)	0.0335 (16)	0.0311 (15)	-0.0003 (13)	0.0032 (12)	0.0010 (12)
C2	0.0297 (16)	0.0302 (16)	0.0340 (16)	0.0005 (13)	-0.0005 (12)	-0.0018 (13)
C3	0.0257 (16)	0.0312 (17)	0.0465 (18)	-0.0024 (13)	0.0041 (13)	0.0057 (14)
C4	0.0324 (17)	0.045 (2)	0.0418 (18)	-0.0003 (15)	0.0138 (14)	0.0039 (15)
C5	0.0307 (16)	0.0435 (18)	0.0351 (16)	0.0013 (15)	0.0087 (13)	-0.0045 (14)
C6	0.0271 (15)	0.0299 (15)	0.0375 (16)	0.0010 (13)	0.0049 (12)	-0.0009 (13)
C7	0.0312 (17)	0.0347 (17)	0.0467 (19)	-0.0006 (14)	0.0069 (14)	-0.0085 (14)
C8	0.0352 (18)	0.0379 (17)	0.0381 (17)	-0.0011 (15)	0.0099 (14)	-0.0005 (14)
C9	0.056 (2)	0.073 (2)	0.0364 (19)	-0.005 (2)	0.0046 (17)	0.0057 (18)
C10	0.052 (2)	0.108 (3)	0.038 (2)	-0.017 (2)	-0.0002 (18)	-0.013 (2)
C11	0.037 (2)	0.068 (2)	0.057 (2)	-0.0145 (19)	0.0128 (17)	-0.029 (2)
C12	0.0336 (18)	0.0393 (18)	0.053 (2)	-0.0167 (15)	0.0122 (15)	-0.0119 (16)
C13	0.0264 (16)	0.0319 (16)	0.0429 (18)	-0.0010 (13)	0.0102 (13)	-0.0019 (13)
C14	0.0333 (17)	0.0346 (18)	0.0422 (18)	-0.0016 (14)	0.0051 (14)	-0.0035 (14)
C15	0.0291 (17)	0.0330 (18)	0.058 (2)	0.0013 (14)	0.0092 (15)	-0.0009 (15)
C16	0.0364 (19)	0.0392 (18)	0.050 (2)	0.0007 (15)	0.0194 (15)	-0.0019 (15)
C17	0.0384 (18)	0.0404 (19)	0.0390 (17)	-0.0040 (15)	0.0143 (14)	0.0007 (14)
C18	0.0313 (17)	0.0377 (17)	0.0369 (17)	-0.0004 (14)	0.0065 (13)	-0.0002 (14)
C19	0.0355 (18)	0.042 (2)	0.0363 (17)	-0.0019 (15)	0.0102 (14)	0.0053 (14)
C20	0.0382 (19)	0.0361 (18)	0.0418 (18)	0.0020 (15)	0.0091 (14)	-0.0008 (14)
C21	0.065 (2)	0.048 (2)	0.045 (2)	-0.007 (2)	0.0110 (18)	-0.0156 (17)
C22	0.053 (2)	0.096 (3)	0.043 (2)	0.003 (2)	-0.0043 (18)	-0.021 (2)
C23	0.043 (2)	0.075 (2)	0.0372 (18)	0.0237 (19)	0.0035 (15)	0.0001 (18)

C24	0.0356 (18)	0.0414 (18)	0.0375 (17)	0.0130 (15)	0.0066 (14)	0.0012 (14)
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Geometric parameters (\AA , $^{\circ}$)

Cu1—O1	1.894 (2)	C18—C19	1.501 (4)
Cu1—O2	1.895 (2)	C20—C21	1.519 (4)
Cu1—N1	2.074 (2)	C21—C22	1.519 (5)
Cu1—N2	2.072 (2)	C22—C23	1.512 (6)
Cl1—C2	1.745 (3)	C23—C24	1.515 (4)
Cl2—C4	1.753 (3)	C3—H1	0.950
Cl3—C14	1.740 (3)	C5—H2	0.950
Cl4—C16	1.745 (3)	C7—H3	0.950
O1—C1	1.320 (3)	C7—H4	0.950
O2—C13	1.316 (3)	C8—H5	0.950
N1—C7	1.490 (3)	C8—H6	0.950
N1—C8	1.500 (4)	C9—H7	0.950
N1—C12	1.501 (3)	C9—H8	0.950
N2—C19	1.490 (4)	C10—H9	0.950
N2—C20	1.498 (3)	C10—H10	0.950
N2—C24	1.495 (3)	C11—H11	0.950
C1—C2	1.403 (4)	C11—H12	0.950
C1—C6	1.405 (4)	C12—H13	0.950
C2—C3	1.379 (4)	C12—H14	0.950
C3—C4	1.383 (4)	C15—H15	0.950
C4—C5	1.369 (4)	C17—H16	0.950
C5—C6	1.390 (4)	C19—H17	0.950
C6—C7	1.496 (4)	C19—H18	0.950
C8—C9	1.519 (4)	C20—H19	0.950
C9—C10	1.531 (6)	C20—H20	0.950
C10—C11	1.504 (5)	C21—H21	0.950
C11—C12	1.518 (4)	C21—H22	0.950
C13—C14	1.397 (4)	C22—H23	0.950
C13—C18	1.411 (4)	C22—H24	0.950
C14—C15	1.392 (4)	C23—H25	0.950
C15—C16	1.378 (4)	C23—H26	0.950
C16—C17	1.375 (4)	C24—H27	0.950
C17—C18	1.381 (4)	C24—H28	0.950
O1—Cu1—O2	166.02 (9)	N1—C7—H3	107.9
O1—Cu1—N1	92.60 (9)	N1—C7—H4	108.0
O1—Cu1—N2	86.99 (9)	C6—C7—H3	107.9
O2—Cu1—N1	88.97 (9)	C6—C7—H4	107.9
O2—Cu1—N2	93.76 (9)	H3—C7—H4	109.5
N1—Cu1—N2	170.32 (9)	N1—C8—H5	107.8
Cu1—O1—C1	130.09 (18)	N1—C8—H6	108.0
Cu1—O2—C13	125.43 (18)	C9—C8—H5	108.9
Cu1—N1—C7	109.01 (17)	C9—C8—H6	108.2
Cu1—N1—C8	104.62 (17)	H5—C8—H6	109.5

Cu1—N1—C12	112.29 (18)	C8—C9—H7	109.0
C7—N1—C8	113.8 (2)	C8—C9—H8	109.6
C7—N1—C12	108.7 (2)	C10—C9—H7	108.9
C8—N1—C12	108.4 (2)	C10—C9—H8	109.3
Cu1—N2—C19	110.63 (17)	H7—C9—H8	109.5
Cu1—N2—C20	106.62 (17)	C9—C10—H9	110.0
Cu1—N2—C24	109.16 (18)	C9—C10—H10	108.8
C19—N2—C20	111.6 (2)	C11—C10—H9	109.9
C19—N2—C24	108.7 (2)	C11—C10—H10	108.3
C20—N2—C24	110.1 (2)	H9—C10—H10	109.5
O1—C1—C2	120.9 (2)	C10—C11—H11	108.3
O1—C1—C6	122.5 (2)	C10—C11—H12	109.7
C2—C1—C6	116.6 (2)	C12—C11—H11	108.6
C11—C2—C1	118.3 (2)	C12—C11—H12	109.8
C11—C2—C3	118.5 (2)	H11—C11—H12	109.5
C1—C2—C3	123.2 (2)	N1—C12—H13	108.6
C2—C3—C4	117.8 (2)	N1—C12—H14	107.8
C12—C4—C3	118.7 (2)	C11—C12—H13	108.1
C12—C4—C5	119.7 (2)	C11—C12—H14	109.0
C3—C4—C5	121.6 (3)	H13—C12—H14	109.5
C4—C5—C6	120.1 (2)	C14—C15—H15	120.8
C1—C6—C5	120.7 (2)	C16—C15—H15	120.7
C1—C6—C7	118.7 (2)	C16—C17—H16	119.4
C5—C6—C7	120.5 (2)	C18—C17—H16	119.8
N1—C7—C6	115.6 (2)	N2—C19—H17	109.0
N1—C8—C9	114.4 (2)	N2—C19—H18	107.6
C8—C9—C10	110.6 (3)	C18—C19—H17	108.5
C9—C10—C11	110.4 (3)	C18—C19—H18	107.7
C10—C11—C12	111.0 (3)	H17—C19—H18	109.5
N1—C12—C11	113.9 (2)	N2—C20—H19	108.5
O2—C13—C14	121.0 (2)	N2—C20—H20	107.9
O2—C13—C18	122.1 (2)	C21—C20—H19	109.1
C14—C13—C18	116.8 (2)	C21—C20—H20	107.9
C13—C14—C13	118.6 (2)	H19—C20—H20	109.5
C13—C14—C15	118.8 (2)	C20—C21—H21	108.4
C13—C14—C15	122.6 (2)	C20—C21—H22	109.5
C14—C15—C16	118.6 (2)	C22—C21—H21	108.1
C14—C16—C15	119.3 (2)	C22—C21—H22	109.9
C14—C16—C17	120.0 (2)	H21—C21—H22	109.5
C15—C16—C17	120.7 (3)	C21—C22—H23	109.9
C16—C17—C18	120.8 (2)	C21—C22—H24	108.4
C13—C18—C17	120.6 (2)	C23—C22—H23	110.0
C13—C18—C19	118.0 (2)	C23—C22—H24	108.3
C17—C18—C19	121.2 (2)	H23—C22—H24	109.5
N2—C19—C18	114.5 (2)	C22—C23—H25	108.1
N2—C20—C21	113.9 (2)	C22—C23—H26	109.9
C20—C21—C22	111.4 (3)	C24—C23—H25	108.6
C21—C22—C23	110.7 (3)	C24—C23—H26	109.8

C22—C23—C24	110.9 (3)	H25—C23—H26	109.5
N2—C24—C23	114.1 (2)	N2—C24—H27	108.5
C2—C3—H1	121.1	N2—C24—H28	107.6
C4—C3—H1	121.0	C23—C24—H27	108.2
C4—C5—H2	119.9	C23—C24—H28	108.9
C6—C5—H2	120.0	H27—C24—H28	109.5
O1—Cu1—O2—C13	65.3 (4)	O1—C1—C6—C5	178.9 (2)
O2—Cu1—O1—C1	87.2 (4)	O1—C1—C6—C7	3.0 (4)
O1—Cu1—N1—C7	−32.33 (19)	C2—C1—C6—C5	1.1 (4)
O1—Cu1—N1—C8	89.75 (18)	C2—C1—C6—C7	−174.9 (2)
O1—Cu1—N1—C12	−152.88 (19)	C6—C1—C2—Cl1	−178.1 (2)
N1—Cu1—O1—C1	−9.0 (2)	C6—C1—C2—C3	0.1 (3)
O1—Cu1—N2—C19	173.93 (19)	Cl1—C2—C3—C4	177.5 (2)
O1—Cu1—N2—C20	−64.57 (19)	C1—C2—C3—C4	−0.7 (4)
O1—Cu1—N2—C24	54.36 (19)	C2—C3—C4—Cl2	179.8 (2)
N2—Cu1—O1—C1	−179.4 (2)	C2—C3—C4—C5	0.1 (3)
O2—Cu1—N1—C7	161.57 (19)	Cl2—C4—C5—C6	−178.6 (2)
O2—Cu1—N1—C8	−76.35 (18)	C3—C4—C5—C6	1.1 (4)
O2—Cu1—N1—C12	41.02 (19)	C4—C5—C6—C1	−1.7 (4)
N1—Cu1—O2—C13	162.0 (2)	C4—C5—C6—C7	174.2 (2)
O2—Cu1—N2—C19	−20.06 (19)	C1—C6—C7—N1	−52.8 (3)
O2—Cu1—N2—C20	101.45 (19)	C5—C6—C7—N1	131.2 (2)
O2—Cu1—N2—C24	−139.62 (19)	N1—C8—C9—C10	−55.2 (4)
N2—Cu1—O2—C13	−27.3 (2)	C8—C9—C10—C11	54.1 (4)
Cu1—O1—C1—C2	−156.2 (2)	C9—C10—C11—C12	−55.0 (4)
Cu1—O1—C1—C6	26.0 (4)	C10—C11—C12—N1	56.8 (3)
Cu1—O2—C13—C14	−142.5 (2)	O2—C13—C14—Cl3	2.8 (4)
Cu1—O2—C13—C18	39.7 (4)	O2—C13—C14—C15	−177.5 (2)
Cu1—N1—C7—C6	64.2 (2)	O2—C13—C18—C17	178.2 (2)
Cu1—N1—C8—C9	173.9 (2)	O2—C13—C18—C19	3.4 (4)
Cu1—N1—C12—C11	−169.4 (2)	C14—C13—C18—C17	0.3 (4)
C7—N1—C8—C9	−67.2 (3)	C14—C13—C18—C19	−174.5 (2)
C8—N1—C7—C6	−52.1 (3)	C18—C13—C14—Cl3	−179.3 (2)
C7—N1—C12—C11	69.9 (3)	C18—C13—C14—C15	0.4 (4)
C12—N1—C7—C6	−173.1 (2)	Cl3—C14—C15—C16	179.3 (2)
C8—N1—C12—C11	−54.3 (3)	C13—C14—C15—C16	−0.3 (4)
C12—N1—C8—C9	53.9 (3)	C14—C15—C16—Cl4	177.8 (2)
Cu1—N2—C19—C18	59.2 (2)	C14—C15—C16—C17	−0.4 (4)
Cu1—N2—C20—C21	170.0 (2)	Cl4—C16—C17—C18	−177.1 (2)
Cu1—N2—C24—C23	−169.5 (2)	C15—C16—C17—C18	1.1 (5)
C19—N2—C20—C21	−69.1 (3)	C16—C17—C18—C13	−1.1 (4)
C20—N2—C19—C18	−59.4 (3)	C16—C17—C18—C19	173.6 (3)
C19—N2—C24—C23	69.8 (3)	C13—C18—C19—N2	−57.2 (3)
C24—N2—C19—C18	179.0 (2)	C17—C18—C19—N2	128.0 (3)
C20—N2—C24—C23	−52.7 (3)	N2—C20—C21—C22	−53.5 (4)
C24—N2—C20—C21	51.7 (3)	C20—C21—C22—C23	53.9 (4)
O1—C1—C2—Cl1	4.0 (3)	C21—C22—C23—C24	−54.5 (4)

supporting information

O1—C1—C2—C3

−177.8 (2)

C22—C23—C24—N2

55.2 (3)
