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Synthesis and crystal structure of the dinuclear copper(II)
Schiff base complex μ -hydroxido- μ -chlorido-bis{[bis(*trans*-2-
nitrocinnamaldehyde)ethylenediamine]chloridocopper(II)}
dichloromethane sesquisolvate

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Synthesis and crystal structure of the dinuclear copper(II) Schiff base complex μ -hydroxido- μ -chlorido-bis{[bis(*trans*-2-nitrocinnamaldehyde)-ethylenediamine]chloridocopper(II)} dichloromethane sesquisolvate

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Transition metal complexes of Schiff base ligands have been shown to have particular application in catalysis and magnetism. The chemistry of copper complexes is of interest owing to their importance in biological and industrial processes. The reaction of copper(I) chloride with the bidentate Schiff base *N,N'*-bis(*trans*-2-nitrocinnamaldehyde)ethylenediamine {Nca₂en, systematic name: (1*E*,1'*E*,2*E*,2'*E*)-*N,N'*-(ethane-1,2-diyl)bis[3-(2-nitrophenyl)prop-2-en-1-imine]} in a 1:1 molar ratio in dichloromethane without exclusion of air or moisture resulted in the formation of the title complex μ -chlorido- μ -hydroxido-bis(chlorido{ (1*E*,1'*E*,2*E*,2'*E*)-*N,N'*-(ethane-1,2-diyl)bis[3-(2-nitrophenyl)prop-2-en-1-imine]- κ^2 *N,N'* }copper(II)) dichloromethane sesquisolvate, [Cu₂Cl₃(OH)-(C₂₀H₁₈N₄O₄)₂].1.5CH₂Cl₂. The dinuclear complex has a folded four-membered ring in an unsymmetrical Cu₂OCl₃ core in which the approximate trigonal bipyramidal coordination displays different angular distortions in the equatorial planes of the two Cu^{II} atoms; the chloride bridge is asymmetric, but the hydroxide bridge is symmetric. The chelate rings of the two Nca₂en ligands have different conformations, leading to a more marked bowing of one of the ligands compared with the other. This is the first reported dinuclear complex, and the first five-coordinate complex, of the Nca₂en Schiff base ligand. Molecules of the dimer are associated in pairs by ring-stacking interactions supported by C—H...Cl interactions with solvent molecules; a further ring-stacking interaction exists between the two Schiff base ligands of each molecule.

1. Introduction

Transition metal complexes of Schiff base ligands have been of interest for many years, with particular application in catalysis and magnetism, and their structures have been investigated extensively (Archer & Wang, 1990; Chang *et al.*, 1998; Chaturvedi, 1997; Costamagna *et al.*, 1992). Since the 2014 Cambridge Structural Database (CSD) search mentioned in our previous report of one particular Schiff base ligand and one of its complexes (Clegg *et al.*, 2015), the number of entries in the CSD (Version 5.37, including one update, November 2015; Allen, 2002; Groom & Allen, 2014) for purely organic compounds containing the skeleton *R*—CH=N—CH₂CH₂—N=CH—*R*, in which *R* is any alkyl or aryl group, has increased to 165 and the number of metal complexes of such ligands to 1872. The chemistry of copper complexes is of

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Table 1
Experimental details.

Crystal data	
Chemical formula	$[\text{Cu}_2\text{Cl}_3(\text{OH})(\text{C}_{20}\text{H}_{18}\text{N}_4\text{O}_4)_2] \cdot 1.5\text{CH}_2\text{Cl}_2$
M_r	1134.59
Crystal system, space group	Monoclinic, $C2/c$
Temperature (K)	150
a, b, c (Å)	33.62 (3), 14.897 (11), 20.948 (16)
β (°)	110.544 (14)
V (Å ³)	9825 (13)
Z	8
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	1.25
Crystal size (mm)	0.34 × 0.30 × 0.30
Data collection	
Diffractometer	Bruker SMART 1K CCD
Absorption correction	Multi-scan (SADABS; Bruker, 2008)
$T_{\min}, T_{\max}$	0.681, 0.710
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	29716, 7672, 4768
R_{int}	0.119
θ_{max} (°)	24.0
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.572
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.067, 0.223, 1.05
No. of reflections	7672
No. of parameters	610
No. of restraints	20
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	0.98, -0.86

Computer programs: SMART (Bruker, 2008), SAINT (Bruker, 2008), SHELXTL (Sheldrick, 2008), SHELXL2014 (Sheldrick, 2015) and local programs.

particular interest owing to their importance in biological and industrial processes (Que & Tolman, 2002). In recent years, metal complexes of Schiff bases have attracted considerable attention due to their antifungal, antibacterial and antitumour activity (Usha & Chandra, 1992; Garg & Kapur, 1990). Biological activities may be related to the redox properties of complexes: for some copper(II) complexes a lower reduction potential seems to be related to an increased antifungal activity (Haiduc & Silvestru, 1990). Mononuclear and dinuclear copper complexes can mimic the abilities of superoxide dismutase (SOD), catechol oxidase and chemical nucleases (Liu *et al.*, 1996). Complexes of copper(II) with Schiff base ligands (Marten *et al.*, 2005) are frequently studied, for example, for their antibacterial properties (You & Zhu, 2006). Dicopper(II) Schiff base and related complexes have been probed electrochemically (Zolezzi *et al.*, 2002), magnetically (Zeyrek *et al.*, 2006) and by electron paramagnetic resonance (EPR) (Griebel *et al.*, 2006) for their electronic structure.

We have continued our exploration of complexes of the ligand *N,N'*-bis(*trans*-2-nitrocinnamaldehyde)ethylenediamine (Nca₂en) and report here its first dinuclear complex, namely $[\text{Cu}_2\text{Cl}_3(\text{OH})(\text{Nca}_2\text{en})_2] \cdot 1.5\text{CH}_2\text{Cl}_2$, (I). The 11 previously reported complexes (referenced in Clegg *et al.*, 2015) of cobalt, nickel, copper, zinc and silver are all mononuclear and four-coordinate, with a single Nca₂en ligand and either one other bidentate or two monodentate ligands, except for the homo-

leptic salt $[\text{Cu}(\text{Nca}_2\text{en})_2]\text{ClO}_4$ (Dehghanpour *et al.*, 2006). The structure reported here thus introduces new features to the series.

2. Experimental

2.1. Synthesis and crystallization

To a stirred solution of CuCl (99 mg, 1 mmol) in dichloromethane (5 ml) was added dropwise at room temperature a solution of *N,N'*-bis(*trans*-2-nitrocinnamaldehyde)ethylenediamine (378 mg, 1 mmol) in dichloromethane (10 ml), and stirring was continued for 1 h. After filtration, the volume of the solution was reduced under vacuum to about 4 ml. Slow diffusion of diethyl ether vapour into this concentrated solution gave yellow crystals suitable for X-ray diffraction, albeit with relatively weak diffraction at higher angles (yield 291 mg, 58%). Analysis calculated for $\text{C}_{40}\text{H}_{37}\text{Cl}_3\text{Cu}_2\text{N}_8\text{O}_9$: C 47.70, H 3.70, N 11.12%; calculated for $\text{C}_{40}\text{H}_{37}\text{Cl}_3\text{Cu}_2\text{N}_8\text{O}_9 \cdot 1.5\text{CH}_2\text{Cl}_2$: C 43.93, H 3.55, N 9.87%; found: C 47.66, H 3.67, N 11.07%. This indicates that the solvent of crystallization was lost in the preparation for analysis following removal from the mother liquor.

2.2. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. One dichloromethane solvent molecule was found to be ordered in a general position, and another lies across a mirror plane with the CH₂ group disordered unequally [0.91 (2):0.09 (2)] over two positions in the mirror plane; similarity restraints were applied to the C—Cl distances and anisotropic displacement parameters of this molecule, and the displacement parameters were also subjected to a 'rigid-bond' restraint. The H atom of the bridging OH ligand was located in a difference map and was refined with the O—H distance restrained to 0.84 (1) Å, but with no constraint or restraint on its isotropic displacement parameter. All other H atoms were included in calculated positions and refined using a riding model, and with $U_{\text{iso}}(\text{H}) =$

Table 2
Selected geometric parameters (Å, °).

Cu1—O1	1.923 (5)	Cu2—O1	1.930 (5)
Cu1—Cl1	2.426 (3)	Cu2—Cl1	2.568 (3)
Cu1—Cl2	2.295 (2)	Cu2—Cl3	2.300 (2)
Cu1—N6	2.168 (6)	Cu2—N2	2.043 (7)
Cu1—N7	1.991 (6)	Cu2—N3	2.012 (6)
O1—Cu1—Cl1	85.14 (15)	O1—Cu2—Cl1	81.13 (15)
O1—Cu1—Cl2	91.30 (16)	O1—Cu2—Cl3	91.73 (16)
O1—Cu1—N6	102.9 (2)	O1—Cu2—N2	94.6 (2)
O1—Cu1—N7	174.7 (2)	O1—Cu2—N3	174.9 (2)
Cl1—Cu1—Cl2	150.99 (9)	Cl1—Cu2—Cl3	112.22 (9)
Cl1—Cu1—N6	104.25 (16)	Cl1—Cu2—N2	112.20 (17)
Cl1—Cu1—N7	91.17 (17)	Cl1—Cu2—N3	99.05 (19)
Cl2—Cu1—N6	104.61 (17)	Cl3—Cu2—N2	135.58 (18)
Cl2—Cu1—N7	90.12 (18)	Cl3—Cu2—N3	92.87 (18)
N6—Cu1—N7	81.6 (2)	N2—Cu2—N3	80.7 (2)
Cu1—O1—Cu2	108.4 (2)	Cu1—Cl1—Cu2	77.44 (6)
N2—Cl10—Cl11—N3	−47.0 (8)	N6—C30—C31—N7	−50.9 (8)

1.2 $U_{eq}(C)$. A number of reflections (amounting to around 30 in the unique set) were rejected during processing of the raw data because of inconsistent intensities; these are likely to have been affected by overlap of diffraction from a minor second crystal component.

3. Results and discussion

The source of the hydroxide ligand in the product of the synthesis is unclear; presumably it is derived from water in one of the reagents, the solvent or the atmosphere, as no precautions were taken to exclude air or moisture.

The dinuclear complex (Fig. 1) has hydroxide and chloride bridges between the two Cu^{II} atoms. Both metal centres have a coordination geometry best described as distorted trigonal bipyramidal, with the axial sites occupied by the O atom of the bridging OH ligand and one N atom (N3 or N7), the interaxial angles being essentially identical and deviating from the ideal value of 180° by only about 5° (Table 2). There is a difference, however, in the pattern of distortions from the ideal angles of 120° in the equatorial planes: at atom Cu1, the Cl1—Cu1—Cl2 angle is significantly expanded to 150.99 (9)°, but at atom Cu2, the widest equatorial angle is Cl3—Cu2—N2 of 135.58 (18)°, and in each case the other two equatorial angles are approximately equal. This difference leads to a marked asymmetry in the central Cu₂OCl₃ core of the complex, which might have been expected to display an approximate mirror plane passing through the bridging ligands; the asymmetry can also be seen in the significantly different Cu—Cl bond lengths to the chloride bridge and in the Cu—N bond lengths to the Schiff base ligands. The τ parameter (Addison *et al.*, 1984) is 0.40 for Cu1 and 0.66 for Cu2, indicating a geometry intermediate between ideal trigonal bipyramidal ($\tau = 1$) and square-based pyramidal ($\tau = 0$), and significantly different for the two metal centres. The closer approach to square-based pyramidal geometry for atom Cu1 is mainly a consequence of the wide Cl1—Cu1—Cl2 angle. The +2 oxidation state is confirmed for both Cu^{II} atoms by bond-valence calculations

(Brese & O'Keeffe, 1991; Brown, 2002), a bond-valence sum of 2.1 being obtained in each case.

The four-membered Cu₂OCl ring is folded, with a dihedral (hinge) angle of 152.0 (3)° between the two OCuCl planes. A search of the CSD for the Cu₂OCl₃ core finds just eight previous examples that are not parts of larger clusters with more than two Cu atoms; all have two five-coordinated Cu^{II} atoms, the other two coordination sites being taken by N atoms of uncharged ligands in each case. Of these, six have a tetradentate ligand that plays both chelating and bridging roles, imposing a marked fold on the central four-membered ring, the hinge angle ranging from 135.6 to 142.7° for phthalazine-based ligands (Marongiu & Lingafelter, 1982; Mandal *et al.*, 1985; Thompson *et al.*, 1987; Chen *et al.*, 1993, 1996) and the more open angle of 159.6° for one 1,8-naphthyridine-based ligand (Tikkanen *et al.*, 1984); the hinge angle is widened to 168.2° for a complex with chelating but nonbridging propylenediamine ligands (Walther *et al.*, 1997) and to 178.9° (virtually planar) for a complex with monodentate pyrazole ligands (Mezei & Raptis, 2004). Within this small set of structures, there is thus a strong correlation between the degree of folding of the four-membered ring and the N—Cu—N bite angle, and bridging geometry restrictions imposed by the N-donor ligands. Interestingly, almost all of

Figure 1
The dinuclear molecule of the title compound, (I), shown with 40% probability displacement ellipsoids. The dichloromethane solvent molecules have been omitted for clarity.

these structures have approximately symmetrical chloride bridges, the difference in the two Cu—Cl bond lengths being less than 0.08 Å, except in the structure with the most similar ligand environment to that of the present compound (Walther *et al.*, 1997), where the distances are 2.507 and 2.648 Å, a difference of 0.141 Å, essentially identical to the one found here; all the hydroxide bridges are approximately symmetrical.

Each of the two Nca₂en ligands has two substituents attached to the central chelate ring, consisting of three essentially planar groups that are twisted relative to each other. In each case, the nitro group and the conjugated N=C—C=C chain are rotated in the same direction (clockwise or anticlockwise) out of the plane of the benzene ring; the dihedral angles between the ring and nitro group range from 15.7 (8) to 34.8 (9)°, and those between the ring and the chain range from 19.7 (7) to 36.8 (6)°. The two ligands differ significantly in the conformation of their chelate rings: the ring containing atom Cu1 is best described as an envelope, with atom C30 as the flap atom displaced from the mean plane of the other four atoms, while the ring containing atom Cu2 is twisted on the N2—C10 bond (these two atoms lie above and below the plane of the other three atoms). This difference contributes further to the asymmetry of the molecule and leads to a much more strongly marked bowing of the Cu2-coordinated ligand.

The planes of the benzene rings containing atoms C15 and C35, one in each of the two ligands, are approximately parallel [dihedral angle = 20.0 (4)°] and sufficiently close together [separation of centroids = 3.915 (6) Å] to indicate a possible weak intramolecular ring-stacking interaction; this can be seen in Fig. 1. More significant interactions are found for rings of the Cu2-coordinated ligand (containing atoms C6 and C15) in pairs of inversion-related cations, with a centroid-centroid separation of 3.730 (6) Å and a dihedral angle of 7.8 (4)°. The space between these two molecules is occupied by two dichloromethane solvent molecules having close contacts with

the two bridging chloride ligands (see *Supporting information* and Fig. 2), which may be considered as C—H...Cl secondary hydrogen-bonding interactions supporting the ring stacking in dimer formation. Other close C—H...X contacts listed in the *Supporting information* involve the terminal chloride ligands and O atoms of the nitro groups.

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References

- Addison, A. W., Rao, T. N., Reedijk, J., van Rijn, J. & Verschoor, G. C. (1984). *J. Chem. Soc. Dalton Trans.* pp. 1349–1356.
- Allen, F. H. (2002). *Acta Cryst.* **B58**, 380–388.
- Archer, R. D. & Wang, B. (1990). *Inorg. Chem.* **29**, 39–43.
- Brese, N. E. & O'Keefe, M. (1991). *Acta Cryst.* **B47**, 192–197.
- Brown, I. D. (2002). In *The Chemical Bond in Inorganic Chemistry: The Bond Valence Model*. Oxford University Press.
- Bruker (2008). *SMART, SAINT and SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Chang, S., Jones, L., Wang, C. M., Henling, L. M. & Grubbs, R. H. (1998). *Organometallics*, **17**, 3460–3465.
- Chaturvedi, K. K. (1997). *J. Inorg. Nucl. Chem.* **39**, 901–903.
- Chen, L., Thompson, L. K. & Bridson, J. N. (1993). *Inorg. Chim. Acta*, **214**, 67–76.
- Chen, L., Thompson, L. K. & Bridson, J. N. (1996). *Inorg. Chim. Acta*, **244**, 87–93.
- Clegg, W., Harrington, R. W., Barati, K., Habibi, M. H., Montazer-ozohori, M. & Lalegani, A. (2015). *Acta Cryst.* **C71**, 578–583.
- Costamagna, J., Vargas, J., Latorre, R., Alvarado, A. & Mena, G. (1992). *Coord. Chem. Rev.* **119**, 67–88.
- Dehghanpour, S., Kempe, R., Balireddi, S., Fotouhi, L., Tabasi, F., Mojahed, F. & Salek, S. (2006). *Z. Anorg. Allg. Chem.* **632**, 2321–2325.
- Garg, B. S. & Kapur, L. (1990). *Inorg. Chim. Acta*, **173**, 223–227.
- Griebel, J., Leistner, F., Krautscheid, H. & Kirmse, R. (2006). *Z. Anorg. Allg. Chem.* **632**, 866–870.
- Groom, C. R. & Allen, F. H. (2014). *Angew. Chem. Int. Ed.* **53**, 662–671.
- Haiduc, I. & Silvestru, A. (1990). *Coord. Chem. Rev.* **99**, 253–296.
- Liu, C. M., Xiong, G., You, X. Z. & Liu, Y. J. (1996). *Polyhedron*, **15**, 4565–4571.
- Mandal, S. K., Thompson, L. K. & Hanson, A. W. (1985). *Chem. Commun.* pp. 1709–1711.
- Marongiu, G. & Lingafelter, E. C. (1982). *Acta Cryst.* **B38**, 620–622.
- Marten, J., Seichter, W. & Weber, E. (2005). *Z. Anorg. Allg. Chem.* **631**, 869–877.
- Mezei, G. & Raptis, R. G. (2004). *Inorg. Chim. Acta*, **357**, 3279–3288.
- Que, L. & Tolman, W. B. (2002). *Angew. Chem.* **114**, 1160–1185.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Sheldrick, G. M. (2015). *Acta Cryst.* **C71**, 3–8.
- Thompson, L. K., Mandal, S. K., Rosenberg, L., Lee, F. L. & Gabe, E. J. (1987). *Inorg. Chim. Acta*, **133**, 81–91.
- Tikkanen, W. R., Krüger, C., Bomben, K. D., Jolly, W. L., Kaska, W. C. & Ford, P. C. (1984). *Inorg. Chem.* **23**, 3633–3638.
- Usha, A. K. & Chandra, S. (1992). *Synth. React. Inorg. Met.-Org. Chem.* **22**, 1565–1579.
- Walther, D., Hamza, K., Gorls, H. & Imhof, W. (1997). *Z. Anorg. Allg. Chem.* **623**, 1135–1143.
- You, Z.-L. & Zhu, H.-L. (2006). *Z. Anorg. Allg. Chem.* **632**, 140–146.
- Zeyrek, C. T., Elmali, A. & Elerman, Y. (2006). *Z. Naturforsch. Teil B*, **61**, 237–242.
- Zolezzi, S., Spodine, E. & Decinti, A. (2002). *Polyhedron*, **21**, 55–59.

Figure 2
Dimer formation in (I) through ring stacking and C—H...Cl interactions with ordered dichloromethane solvent molecules.

supporting information

Acta Cryst. (2016). **C72**, 239–242 [doi:10.1107/S2053229616003144]

Synthesis and crystal structure of the dinuclear copper(II) Schiff base complex μ -hydroxido- μ -chlorido-bis{[bis(*trans*-2-nitrocinnamaldehyde)ethylenediamine]-chloridocopper(II)} dichloromethane sesquisolvate

Kazem Barati, William Clegg, Mohammad Hossein Habibi, Ross W. Harrington, Arash Lalegani and Morteza Montazerzohori

Computing details

Data collection: *SMART* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT* (Bruker, 2008); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL2014* (Sheldrick, 2015) and local programs.

μ -Chlorido- μ -hydroxido-bis(chlorido{(*1E,1'E,2E,2'E*)-*N,N'*-(ethane-1,2-diyl)bis[3-(2-nitrophenyl)prop-2-en-1-imine]- κ^2N,N' })copper(II)) dichloromethane sesquisolvate

Crystal data

[Cu₂Cl₃(OH)(C₂₀H₁₈N₄O₄)₂] $\cdot$ 1.5CH₂Cl₂
 M_r = 1134.59
 Monoclinic, *C2/c*
 a = 33.62 (3) Å
 b = 14.897 (11) Å
 c = 20.948 (16) Å
 β = 110.544 (14)°
 V = 9825 (13) Å³
 Z = 8

$F(000)$ = 4616
 D_x = 1.534 Mg m⁻³
 Mo $K\alpha$ radiation, λ = 0.71073 Å
 Cell parameters from 7202 reflections
 θ = 2.3–26.2°
 μ = 1.25 mm⁻¹
 T = 150 K
 Block, yellow
 0.34 $\times$ 0.30 $\times$ 0.30 mm

Data collection

Bruker SMART 1K CCD
 diffractometer
 Radiation source: sealed tube
 thin-slice ω scans
 Absorption correction: multi-scan
 (*SADABS*; Bruker, 2008)
 $T_{\min}$ = 0.681, $T_{\max}$ = 0.710
 29716 measured reflections

7672 independent reflections
 4768 reflections with $I > 2\sigma(I)$
 R_{int} = 0.119
 $\theta_{\max}$ = 24.0°, $\theta_{\min}$ = 1.5°
 h = -38 $\rightarrow$ 38
 k = -17 $\rightarrow$ 17
 l = -23 $\rightarrow$ 23

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)]$ = 0.067
 $wR(F^2)$ = 0.223
 S = 1.05

7672 reflections
 610 parameters
 20 restraints
 Primary atom site location: structure-invariant
 direct methods

Secondary atom site location: difference Fourier map
 Hydrogen site location: mixed
 H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.1276P)^2]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.98 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.86 \text{ e } \text{\AA}^{-3}$

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 ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Cu1	0.25480 (3)	0.56019 (5)	0.30938 (5)	0.0282 (3)	
Cu2	0.22336 (3)	0.42622 (5)	0.39632 (4)	0.0282 (3)	
O1	0.21615 (16)	0.4631 (3)	0.3046 (2)	0.0308 (12)	
H1	0.219 (3)	0.420 (4)	0.282 (4)	0.05 (3)*	
Cl1	0.25122 (6)	0.58769 (11)	0.42137 (10)	0.0361 (5)	
Cl2	0.28260 (8)	0.48552 (12)	0.23880 (13)	0.0586 (7)	
Cl3	0.27602 (6)	0.32646 (12)	0.39843 (10)	0.0393 (5)	
N1	0.0210 (3)	0.6736 (5)	0.1857 (4)	0.059 (2)	
O2	−0.0133 (2)	0.7131 (5)	0.1626 (4)	0.075 (2)	
O3	0.0233 (3)	0.5912 (5)	0.1863 (5)	0.109 (3)	
N2	0.1597 (2)	0.4179 (4)	0.3787 (3)	0.0353 (15)	
N3	0.22556 (19)	0.3912 (4)	0.4903 (3)	0.0341 (15)	
N4	0.4020 (2)	0.3775 (4)	0.7412 (4)	0.0469 (18)	
O4	0.4245 (2)	0.3797 (4)	0.8024 (3)	0.0597 (17)	
O5	0.3769 (2)	0.3158 (4)	0.7156 (3)	0.0616 (18)	
C1	0.0607 (3)	0.7258 (5)	0.2093 (4)	0.0383 (19)	
C2	0.0608 (3)	0.8054 (6)	0.1754 (5)	0.051 (2)	
H2	0.0363	0.8246	0.1389	0.061*	
C3	0.0974 (4)	0.8561 (6)	0.1960 (6)	0.062 (3)	
H3	0.0987	0.9094	0.1720	0.075*	
C4	0.1321 (3)	0.8302 (5)	0.2512 (6)	0.056 (3)	
H4	0.1565	0.8677	0.2660	0.068*	
C5	0.1320 (3)	0.7505 (5)	0.2854 (4)	0.0393 (19)	
H5	0.1562	0.7339	0.3235	0.047*	
C6	0.0961 (3)	0.6942 (5)	0.2638 (4)	0.039 (2)	
C7	0.0958 (3)	0.6082 (5)	0.2973 (4)	0.0369 (19)	
H7	0.0703	0.5892	0.3031	0.044*	
C8	0.1306 (2)	0.5544 (5)	0.3203 (4)	0.0343 (18)	
H8	0.1562	0.5710	0.3137	0.041*	
C9	0.1284 (2)	0.4719 (5)	0.3551 (4)	0.0380 (19)	

H9	0.1024	0.4571	0.3608	0.046*
C10	0.1551 (3)	0.3383 (5)	0.4178 (5)	0.047 (2)
H10A	0.1645	0.2831	0.4008	0.056*
H10B	0.1253	0.3307	0.4149	0.056*
C11	0.1842 (2)	0.3590 (6)	0.4917 (4)	0.047 (2)
H11A	0.1711	0.4055	0.5116	0.057*
H11B	0.1884	0.3042	0.5200	0.057*
C12	0.2555 (2)	0.3938 (5)	0.5468 (4)	0.0344 (18)
H12	0.2500	0.3716	0.5854	0.041*
C13	0.2977 (2)	0.4281 (4)	0.5578 (4)	0.0316 (17)
H13	0.3055	0.4453	0.5202	0.038*
C14	0.3257 (2)	0.4354 (4)	0.6218 (4)	0.0322 (18)
H14	0.3178	0.4113	0.6576	0.039*
C15	0.3681 (2)	0.4782 (5)	0.6406 (4)	0.0328 (18)
C16	0.3722 (3)	0.5530 (5)	0.6031 (4)	0.0367 (19)
H16	0.3489	0.5711	0.5643	0.044*
C17	0.4103 (3)	0.6016 (5)	0.6221 (4)	0.046 (2)
H17	0.4126	0.6523	0.5961	0.055*
C18	0.4450 (3)	0.5755 (5)	0.6795 (4)	0.046 (2)
H18	0.4710	0.6078	0.6918	0.055*
C19	0.4411 (3)	0.5023 (5)	0.7182 (4)	0.043 (2)
H19	0.4642	0.4848	0.7576	0.052*
C20	0.4028 (3)	0.4551 (5)	0.6981 (4)	0.0360 (19)
N5	0.0608 (3)	0.5335 (6)	−0.0240 (4)	0.061 (2)
O6	0.0313 (4)	0.5281 (7)	−0.0756 (5)	0.142 (4)
O7	0.0865 (3)	0.5890 (5)	−0.0194 (4)	0.087 (2)
N6	0.21390 (19)	0.6619 (4)	0.2452 (3)	0.0279 (14)
N7	0.2979 (2)	0.6568 (4)	0.3229 (3)	0.0280 (14)
N8	0.4795 (2)	0.5391 (4)	0.5511 (3)	0.0388 (16)
O8	0.51637 (19)	0.5214 (4)	0.5873 (3)	0.0572 (17)
O9	0.46738 (19)	0.6159 (4)	0.5332 (3)	0.0513 (15)
C21	0.0666 (3)	0.4692 (6)	0.0326 (4)	0.045 (2)
C22	0.0439 (3)	0.3901 (7)	0.0139 (6)	0.069 (3)
H22	0.0254	0.3819	−0.0319	0.083*
C23	0.0478 (3)	0.3240 (6)	0.0604 (7)	0.071 (3)
H23	0.0324	0.2694	0.0479	0.085*
C24	0.0755 (3)	0.3388 (6)	0.1279 (6)	0.066 (3)
H24	0.0788	0.2941	0.1618	0.079*
C25	0.0982 (3)	0.4196 (5)	0.1449 (5)	0.047 (2)
H25	0.1168	0.4280	0.1906	0.056*
C26	0.0948 (3)	0.4871 (5)	0.0989 (4)	0.0385 (19)
C27	0.1191 (3)	0.5714 (5)	0.1203 (4)	0.0356 (19)
H27	0.1068	0.6256	0.0981	0.043*
C28	0.1573 (3)	0.5754 (5)	0.1691 (4)	0.0356 (19)
H28	0.1701	0.5209	0.1900	0.043*
C29	0.1803 (2)	0.6587 (5)	0.1920 (4)	0.0320 (18)
H29	0.1701	0.7122	0.1668	0.038*
C30	0.2353 (2)	0.7484 (4)	0.2670 (4)	0.0341 (18)

H30A	0.2317	0.7686	0.3096	0.041*	
H30B	0.2231	0.7945	0.2314	0.041*	
C31	0.2826 (2)	0.7345 (5)	0.2787 (4)	0.0378 (19)	
H31A	0.2865	0.7244	0.2345	0.045*	
H31B	0.2989	0.7886	0.3002	0.045*	
C32	0.3368 (3)	0.6516 (5)	0.3599 (4)	0.0359 (19)	
H32	0.3556	0.6988	0.3590	0.043*	
C33	0.3536 (2)	0.5725 (5)	0.4048 (4)	0.0372 (19)	
H33	0.3335	0.5328	0.4124	0.045*	
C34	0.3942 (3)	0.5537 (5)	0.4348 (4)	0.0368 (19)	
H34	0.4144	0.5949	0.4296	0.044*	
C35	0.4100 (2)	0.4737 (5)	0.4753 (4)	0.0342 (18)	
C36	0.3849 (3)	0.3962 (5)	0.4600 (4)	0.041 (2)	
H36	0.3583	0.3980	0.4236	0.049*	
C37	0.3975 (3)	0.3172 (5)	0.4960 (5)	0.047 (2)	
H37	0.3790	0.2668	0.4842	0.056*	
C38	0.4358 (3)	0.3093 (6)	0.5482 (5)	0.060 (3)	
H38	0.4438	0.2543	0.5722	0.072*	
C39	0.4632 (3)	0.3838 (5)	0.5658 (4)	0.047 (2)	
H39	0.4900	0.3805	0.6016	0.056*	
C40	0.4493 (2)	0.4641 (5)	0.5283 (4)	0.0340 (18)	
C41	0.3071 (4)	0.8150 (6)	0.4835 (6)	0.080 (4)	
H41A	0.2944	0.7553	0.4682	0.096*	
H41B	0.2993	0.8334	0.5230	0.096*	
Cl4	0.36367 (10)	0.8074 (2)	0.50904 (19)	0.0970 (10)	
Cl5	0.28670 (12)	0.89185 (19)	0.41790 (16)	0.0938 (10)	
C42	0.0000	0.3843 (12)	0.2500	0.109 (8)	0.91 (2)
H42A	−0.0016	0.4232	0.2874	0.131*	0.454 (11)
H42B	0.0016	0.4232	0.2126	0.131*	0.454 (11)
C42'	0.0000	0.243 (3)	0.2500	0.110 (18)	0.09 (2)
H42C	0.0016	0.2041	0.2126	0.132*	0.046 (11)
H42D	−0.0016	0.2041	0.2874	0.132*	0.046 (11)
Cl6	0.04555 (12)	0.3145 (2)	0.2798 (2)	0.1118 (12)	

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0355 (5)	0.0190 (4)	0.0315 (6)	0.0024 (4)	0.0136 (4)	0.0041 (4)
Cu2	0.0303 (5)	0.0250 (5)	0.0287 (5)	0.0026 (4)	0.0098 (4)	0.0073 (4)
O1	0.047 (3)	0.019 (2)	0.026 (3)	0.000 (2)	0.013 (3)	0.000 (2)
Cl1	0.0514 (12)	0.0251 (9)	0.0390 (12)	−0.0047 (8)	0.0247 (10)	−0.0023 (8)
Cl2	0.0998 (19)	0.0244 (10)	0.0821 (18)	−0.0003 (11)	0.0700 (16)	−0.0042 (10)
Cl3	0.0456 (12)	0.0321 (10)	0.0400 (12)	0.0116 (9)	0.0148 (10)	0.0055 (8)
N1	0.061 (5)	0.041 (5)	0.063 (6)	0.016 (4)	0.006 (4)	0.010 (4)
O2	0.054 (4)	0.065 (4)	0.096 (6)	0.017 (4)	0.014 (4)	0.016 (4)
O3	0.087 (6)	0.038 (4)	0.150 (9)	0.009 (4)	−0.022 (6)	−0.014 (5)
N2	0.043 (4)	0.029 (3)	0.033 (4)	0.002 (3)	0.012 (3)	0.013 (3)
N3	0.030 (4)	0.036 (4)	0.035 (4)	0.004 (3)	0.010 (3)	0.011 (3)

N4	0.051 (5)	0.029 (4)	0.053 (5)	−0.010 (3)	0.008 (4)	−0.004 (3)
O4	0.074 (5)	0.054 (4)	0.041 (4)	−0.012 (3)	0.008 (4)	0.004 (3)
O5	0.075 (5)	0.036 (3)	0.059 (4)	−0.002 (3)	0.004 (4)	0.012 (3)
C1	0.044 (5)	0.027 (4)	0.046 (5)	0.005 (4)	0.018 (4)	−0.002 (4)
C2	0.067 (6)	0.040 (5)	0.057 (6)	0.019 (5)	0.036 (5)	0.004 (4)
C3	0.102 (9)	0.033 (5)	0.084 (8)	0.027 (6)	0.074 (7)	0.020 (5)
C4	0.059 (6)	0.030 (5)	0.100 (8)	0.001 (4)	0.052 (6)	−0.003 (5)
C5	0.040 (5)	0.036 (4)	0.042 (5)	0.010 (4)	0.014 (4)	0.005 (4)
C6	0.049 (5)	0.021 (4)	0.055 (6)	0.012 (4)	0.029 (5)	0.005 (4)
C7	0.040 (5)	0.035 (4)	0.038 (5)	0.001 (4)	0.017 (4)	0.004 (4)
C8	0.031 (4)	0.034 (4)	0.036 (5)	0.010 (3)	0.009 (4)	0.009 (3)
C9	0.032 (5)	0.037 (4)	0.047 (5)	0.004 (4)	0.016 (4)	0.012 (4)
C10	0.039 (5)	0.031 (4)	0.066 (6)	−0.001 (4)	0.013 (5)	0.020 (4)
C11	0.034 (5)	0.058 (5)	0.052 (6)	0.004 (4)	0.019 (4)	0.025 (4)
C12	0.043 (5)	0.031 (4)	0.033 (5)	0.003 (4)	0.018 (4)	0.007 (3)
C13	0.037 (5)	0.030 (4)	0.029 (5)	0.002 (3)	0.013 (4)	−0.003 (3)
C14	0.045 (5)	0.028 (4)	0.028 (5)	0.005 (3)	0.019 (4)	−0.001 (3)
C15	0.039 (5)	0.030 (4)	0.030 (4)	0.002 (3)	0.013 (4)	−0.010 (3)
C16	0.046 (5)	0.034 (4)	0.031 (5)	0.005 (4)	0.014 (4)	−0.006 (3)
C17	0.065 (6)	0.041 (5)	0.042 (5)	0.003 (4)	0.031 (5)	−0.001 (4)
C18	0.049 (5)	0.046 (5)	0.046 (6)	−0.015 (4)	0.022 (5)	−0.012 (4)
C19	0.044 (5)	0.039 (5)	0.041 (5)	0.000 (4)	0.008 (4)	−0.009 (4)
C20	0.050 (5)	0.027 (4)	0.035 (5)	−0.004 (4)	0.021 (4)	−0.004 (3)
N5	0.063 (6)	0.067 (5)	0.044 (5)	−0.026 (5)	0.008 (5)	−0.013 (4)
O6	0.157 (9)	0.140 (9)	0.078 (7)	−0.058 (8)	−0.020 (7)	0.019 (6)
O7	0.118 (7)	0.073 (5)	0.056 (5)	−0.032 (5)	0.014 (5)	0.003 (4)
N6	0.034 (4)	0.021 (3)	0.031 (4)	0.006 (3)	0.016 (3)	0.004 (3)
N7	0.035 (4)	0.026 (3)	0.024 (3)	0.001 (3)	0.011 (3)	0.003 (3)
N8	0.036 (4)	0.040 (4)	0.041 (4)	−0.010 (3)	0.015 (4)	−0.011 (3)
O8	0.031 (4)	0.053 (4)	0.074 (5)	−0.006 (3)	0.002 (3)	−0.011 (3)
O9	0.057 (4)	0.030 (3)	0.067 (4)	−0.008 (3)	0.022 (3)	−0.001 (3)
C21	0.049 (5)	0.047 (5)	0.042 (5)	−0.006 (4)	0.020 (5)	0.005 (4)
C22	0.061 (7)	0.065 (7)	0.083 (8)	−0.026 (5)	0.026 (6)	−0.018 (6)
C23	0.074 (7)	0.044 (6)	0.108 (10)	−0.026 (5)	0.049 (7)	−0.022 (6)
C24	0.087 (8)	0.033 (5)	0.093 (9)	−0.004 (5)	0.051 (7)	−0.006 (5)
C25	0.059 (6)	0.033 (4)	0.053 (6)	−0.001 (4)	0.025 (5)	0.004 (4)
C26	0.049 (5)	0.031 (4)	0.040 (5)	0.002 (4)	0.021 (4)	0.003 (4)
C27	0.049 (5)	0.026 (4)	0.028 (5)	0.003 (4)	0.009 (4)	0.002 (3)
C28	0.049 (5)	0.026 (4)	0.034 (5)	0.003 (4)	0.017 (4)	0.003 (3)
C29	0.047 (5)	0.029 (4)	0.022 (4)	0.013 (4)	0.014 (4)	0.009 (3)
C30	0.043 (5)	0.019 (4)	0.042 (5)	0.005 (3)	0.017 (4)	0.005 (3)
C31	0.049 (5)	0.027 (4)	0.039 (5)	0.004 (4)	0.017 (4)	0.008 (3)
C32	0.046 (5)	0.030 (4)	0.039 (5)	−0.008 (4)	0.024 (4)	0.000 (4)
C33	0.035 (5)	0.035 (4)	0.039 (5)	0.000 (4)	0.010 (4)	0.009 (4)
C34	0.042 (5)	0.034 (4)	0.038 (5)	0.000 (4)	0.018 (4)	−0.003 (4)
C35	0.038 (5)	0.036 (4)	0.033 (5)	−0.006 (4)	0.018 (4)	−0.003 (3)
C36	0.034 (5)	0.035 (4)	0.056 (6)	−0.006 (4)	0.019 (4)	−0.001 (4)
C37	0.047 (5)	0.032 (4)	0.055 (6)	−0.013 (4)	0.010 (5)	0.004 (4)

C38	0.080 (7)	0.038 (5)	0.065 (7)	0.003 (5)	0.029 (6)	0.018 (5)
C39	0.050 (6)	0.045 (5)	0.043 (5)	−0.003 (4)	0.015 (5)	0.001 (4)
C40	0.035 (5)	0.027 (4)	0.042 (5)	−0.003 (3)	0.016 (4)	−0.003 (3)
C41	0.133 (10)	0.049 (6)	0.091 (9)	0.006 (6)	0.080 (8)	−0.001 (6)
Cl4	0.095 (2)	0.088 (2)	0.115 (3)	0.0090 (18)	0.046 (2)	0.0016 (19)
Cl5	0.142 (3)	0.0618 (17)	0.076 (2)	0.0238 (18)	0.036 (2)	−0.0086 (15)
C42	0.046 (9)	0.062 (10)	0.20 (2)	0.000	0.019 (9)	0.000
C42'	0.096 (14)	0.104 (18)	0.13 (4)	0.000	0.037 (15)	0.000
Cl6	0.100 (3)	0.099 (2)	0.139 (3)	0.009 (2)	0.045 (2)	−0.006 (2)

Geometric parameters (Å, °)

Cu1—O1	1.923 (5)	N5—O7	1.176 (9)
Cu1—Cl1	2.426 (3)	N5—C21	1.482 (12)
Cu1—Cl2	2.295 (2)	N6—C29	1.280 (9)
Cu1—N6	2.168 (6)	N6—C30	1.468 (9)
Cu1—N7	1.991 (6)	N7—C31	1.458 (9)
Cu2—O1	1.930 (5)	N7—C32	1.269 (9)
Cu2—Cl1	2.568 (3)	N8—O8	1.234 (8)
Cu2—Cl3	2.300 (2)	N8—O9	1.228 (8)
Cu2—N2	2.043 (7)	N8—C40	1.471 (9)
Cu2—N3	2.012 (6)	C21—C22	1.385 (12)
O1—H1	0.837 (10)	C21—C26	1.406 (12)
N1—O2	1.234 (9)	C22—H22	0.950
N1—O3	1.230 (9)	C22—C23	1.359 (15)
N1—C1	1.472 (11)	C23—H23	0.950
N2—C9	1.280 (9)	C23—C24	1.411 (15)
N2—C10	1.480 (9)	C24—H24	0.950
N3—C11	1.480 (9)	C24—C25	1.403 (12)
N3—C12	1.257 (9)	C25—H25	0.950
N4—O4	1.239 (9)	C25—C26	1.370 (11)
N4—O5	1.237 (8)	C26—C27	1.479 (10)
N4—C20	1.472 (10)	C27—H27	0.950
C1—C2	1.383 (11)	C27—C28	1.332 (11)
C1—C6	1.411 (11)	C28—H28	0.950
C2—H2	0.950	C28—C29	1.452 (10)
C2—C3	1.377 (13)	C29—H29	0.950
C3—H3	0.950	C30—H30A	0.990
C3—C4	1.378 (14)	C30—H30B	0.990
C4—H4	0.950	C30—C31	1.534 (10)
C4—C5	1.388 (11)	C31—H31A	0.990
C5—H5	0.950	C31—H31B	0.990
C5—C6	1.408 (11)	C32—H32	0.950
C6—C7	1.463 (10)	C32—C33	1.489 (10)
C7—H7	0.950	C33—H33	0.950
C7—C8	1.360 (10)	C33—C34	1.318 (11)
C8—H8	0.950	C34—H34	0.950
C8—C9	1.444 (10)	C34—C35	1.450 (10)

C9—H9	0.950	C35—C36	1.399 (10)
C10—H10A	0.990	C35—C40	1.405 (11)
C10—H10B	0.990	C36—H36	0.950
C10—C11	1.543 (12)	C36—C37	1.382 (11)
C11—H11A	0.990	C37—H37	0.950
C11—H11B	0.990	C37—C38	1.373 (12)
C12—H12	0.950	C38—H38	0.950
C12—C13	1.448 (10)	C38—C39	1.405 (12)
C13—H13	0.950	C39—H39	0.950
C13—C14	1.346 (10)	C39—C40	1.417 (11)
C14—H14	0.950	C41—H41A	0.990
C14—C15	1.482 (10)	C41—H41B	0.990
C15—C16	1.396 (10)	C41—C14	1.790 (12)
C15—C20	1.396 (11)	C41—C15	1.734 (11)
C16—H16	0.950	C42—H42A	0.990
C16—C17	1.401 (11)	C42—H42B	0.990
C17—H17	0.950	C42—Cl6	1.774 (11)
C17—C18	1.405 (12)	C42—Cl6 ⁱ	1.774 (11)
C18—H18	0.950	C42'—H42C	0.990
C18—C19	1.392 (11)	C42'—H42D	0.990
C19—H19	0.950	C42'—Cl6	1.79 (2)
C19—C20	1.397 (11)	C42'—Cl6 ⁱ	1.79 (2)
N5—O6	1.186 (11)		
O1—Cu1—Cl1	85.14 (15)	N4—C20—C15	122.2 (7)
O1—Cu1—Cl2	91.30 (16)	N4—C20—C19	115.2 (7)
O1—Cu1—N6	102.9 (2)	C15—C20—C19	122.6 (7)
O1—Cu1—N7	174.7 (2)	O6—N5—O7	118.6 (10)
Cl1—Cu1—Cl2	150.99 (9)	O6—N5—C21	121.2 (9)
Cl1—Cu1—N6	104.25 (16)	O7—N5—C21	120.1 (8)
Cl1—Cu1—N7	91.17 (17)	Cu1—N6—C29	133.5 (5)
Cl2—Cu1—N6	104.61 (17)	Cu1—N6—C30	106.6 (4)
Cl2—Cu1—N7	90.12 (18)	C29—N6—C30	119.4 (6)
N6—Cu1—N7	81.6 (2)	Cu1—N7—C31	114.0 (5)
Cu1—O1—Cu2	108.4 (2)	Cu1—N7—C32	125.9 (5)
Cu1—O1—H1	113 (6)	C31—N7—C32	119.7 (6)
Cu2—O1—H1	111 (6)	O8—N8—O9	122.7 (7)
O1—Cu2—Cl1	81.13 (15)	O8—N8—C40	117.9 (7)
O1—Cu2—Cl3	91.73 (16)	O9—N8—C40	119.4 (7)
O1—Cu2—N2	94.6 (2)	N5—C21—C22	114.7 (9)
O1—Cu2—N3	174.9 (2)	N5—C21—C26	121.4 (7)
Cl1—Cu2—Cl3	112.22 (9)	C22—C21—C26	123.7 (9)
Cl1—Cu2—N2	112.20 (17)	C21—C22—H22	119.7
Cl1—Cu2—N3	99.05 (19)	C21—C22—C23	120.6 (10)
Cl3—Cu2—N2	135.58 (18)	H22—C22—C23	119.7
Cl3—Cu2—N3	92.87 (18)	C22—C23—H23	121.0
N2—Cu2—N3	80.7 (2)	C22—C23—C24	118.0 (9)
Cu1—Cl1—Cu2	77.44 (6)	H23—C23—C24	121.0

O2—N1—O3	121.9 (8)	C23—C24—H24	120.1
O2—N1—C1	119.5 (7)	C23—C24—C25	119.8 (9)
O3—N1—C1	118.5 (8)	H24—C24—C25	120.1
Cu2—N2—C9	134.4 (5)	C24—C25—H25	118.4
Cu2—N2—C10	104.7 (5)	C24—C25—C26	123.3 (9)
C9—N2—C10	119.1 (6)	H25—C25—C26	118.4
Cu2—N3—C11	113.0 (5)	C21—C26—C25	114.6 (7)
Cu2—N3—C12	131.0 (5)	C21—C26—C27	124.8 (7)
C11—N3—C12	116.0 (7)	C25—C26—C27	120.6 (8)
O4—N4—O5	122.9 (7)	C26—C27—H27	118.3
O4—N4—C20	118.5 (6)	C26—C27—C28	123.4 (7)
O5—N4—C20	118.4 (7)	H27—C27—C28	118.3
N1—C1—C2	116.6 (8)	C27—C28—H28	118.4
N1—C1—C6	120.3 (7)	C27—C28—C29	123.3 (7)
C2—C1—C6	123.2 (8)	H28—C28—C29	118.4
C1—C2—H2	120.9	N6—C29—C28	121.6 (7)
C1—C2—C3	118.2 (9)	N6—C29—H29	119.2
H2—C2—C3	120.9	C28—C29—H29	119.2
C2—C3—H3	119.7	N6—C30—H30A	110.2
C2—C3—C4	120.6 (8)	N6—C30—H30B	110.2
H3—C3—C4	119.7	N6—C30—C31	107.4 (6)
C3—C4—H4	119.4	H30A—C30—H30B	108.5
C3—C4—C5	121.2 (9)	H30A—C30—C31	110.2
H4—C4—C5	119.4	H30B—C30—C31	110.2
C4—C5—H5	120.0	N7—C31—C30	108.9 (6)
C4—C5—C6	120.0 (8)	N7—C31—H31A	109.9
H5—C5—C6	120.0	N7—C31—H31B	109.9
C1—C6—C5	116.6 (7)	C30—C31—H31A	109.9
C1—C6—C7	122.3 (7)	C30—C31—H31B	109.9
C5—C6—C7	121.2 (7)	H31A—C31—H31B	108.3
C6—C7—H7	118.8	N7—C32—H32	119.5
C6—C7—C8	122.4 (7)	N7—C32—C33	121.0 (7)
H7—C7—C8	118.8	H32—C32—C33	119.5
C7—C8—H8	120.4	C32—C33—H33	117.7
C7—C8—C9	119.3 (7)	C32—C33—C34	124.6 (7)
H8—C8—C9	120.4	H33—C33—C34	117.7
N2—C9—C8	123.2 (7)	C33—C34—H34	118.0
N2—C9—H9	118.4	C33—C34—C35	123.9 (7)
C8—C9—H9	118.4	H34—C34—C35	118.0
N2—C10—H10A	110.9	C34—C35—C36	118.5 (7)
N2—C10—H10B	110.9	C34—C35—C40	126.5 (7)
N2—C10—C11	104.1 (6)	C36—C35—C40	115.0 (7)
H10A—C10—H10B	109.0	C35—C36—H36	118.9
H10A—C10—C11	110.9	C35—C36—C37	122.2 (8)
H10B—C10—C11	110.9	H36—C36—C37	118.9
N3—C11—C10	108.3 (7)	C36—C37—H37	119.0
N3—C11—H11A	110.0	C36—C37—C38	122.0 (8)
N3—C11—H11B	110.0	H37—C37—C38	119.0

C10—C11—H11A	110.0	C37—C38—H38	120.4
C10—C11—H11B	110.0	C37—C38—C39	119.1 (8)
H11A—C11—H11B	108.4	H38—C38—C39	120.4
N3—C12—H12	117.4	C38—C39—H39	121.2
N3—C12—C13	125.2 (7)	C38—C39—C40	117.6 (8)
H12—C12—C13	117.4	H39—C39—C40	121.2
C12—C13—H13	120.3	N8—C40—C35	122.0 (7)
C12—C13—C14	119.5 (7)	N8—C40—C39	114.0 (7)
H13—C13—C14	120.3	C35—C40—C39	124.0 (7)
C13—C14—H14	117.6	H41A—C41—H41B	108.0
C13—C14—C15	124.8 (7)	H41A—C41—C14	109.4
H14—C14—C15	117.6	H41A—C41—C15	109.4
C14—C15—C16	118.0 (7)	H41B—C41—C14	109.4
C14—C15—C20	123.9 (7)	H41B—C41—C15	109.4
C16—C15—C20	117.6 (7)	C14—C41—C15	111.2 (6)
C15—C16—H16	119.5	H42A—C42—H42B	108.4
C15—C16—C17	121.0 (8)	H42A—C42—C16	110.1
H16—C16—C17	119.5	H42A—C42—C16 ⁱ	110.1
C16—C17—H17	120.0	H42B—C42—C16	110.1
C16—C17—C18	120.1 (8)	H42B—C42—C16 ⁱ	110.1
H17—C17—C18	120.0	C16—C42—C16 ⁱ	108.2 (9)
C17—C18—H18	120.1	H42C—C42'—H42D	108.6
C17—C18—C19	119.8 (8)	H42C—C42'—C16	110.4
H18—C18—C19	120.1	H42C—C42'—C16 ⁱ	110.4
C18—C19—H19	120.5	H42D—C42'—C16	110.4
C18—C19—C20	118.9 (8)	H42D—C42'—C16 ⁱ	110.4
H19—C19—C20	120.5	C16—C42'—C16 ⁱ	107 (2)
O2—N1—C1—C2	−32.0 (12)	O6—N5—C21—C22	19.0 (14)
O2—N1—C1—C6	147.9 (8)	O6—N5—C21—C26	−164.1 (11)
O3—N1—C1—C2	144.1 (9)	O7—N5—C21—C22	−158.2 (9)
O3—N1—C1—C6	−36.0 (13)	O7—N5—C21—C26	18.8 (13)
N1—C1—C2—C3	−180.0 (7)	N5—C21—C22—C23	177.2 (9)
C6—C1—C2—C3	0.0 (12)	C26—C21—C22—C23	0.4 (15)
C1—C2—C3—C4	−3.3 (12)	C21—C22—C23—C24	0.2 (15)
C2—C3—C4—C5	3.2 (13)	C22—C23—C24—C25	−0.5 (15)
C3—C4—C5—C6	0.3 (12)	C23—C24—C25—C26	0.4 (14)
C4—C5—C6—C1	−3.3 (11)	C24—C25—C26—C21	0.1 (12)
C4—C5—C6—C7	177.6 (7)	C24—C25—C26—C27	179.0 (8)
N1—C1—C6—C5	−176.8 (7)	N5—C21—C26—C25	−177.1 (8)
N1—C1—C6—C7	2.3 (11)	N5—C21—C26—C27	4.1 (13)
C2—C1—C6—C5	3.2 (11)	C22—C21—C26—C25	−0.5 (12)
C2—C1—C6—C7	−177.7 (7)	C22—C21—C26—C27	−179.3 (8)
C1—C6—C7—C8	143.7 (8)	C21—C26—C27—C28	−148.9 (8)
C5—C6—C7—C8	−37.2 (11)	C25—C26—C27—C28	32.4 (12)
C6—C7—C8—C9	177.8 (7)	C26—C27—C28—C29	−177.4 (7)
Cu2—N2—C9—C8	13.5 (13)	Cu1—N6—C29—C28	11.3 (11)
C10—N2—C9—C8	175.7 (7)	C30—N6—C29—C28	−178.5 (6)

C7—C8—C9—N2	−179.7 (8)	C27—C28—C29—N6	169.9 (7)
Cu2—N2—C10—C11	57.0 (7)	Cu1—N6—C30—C31	42.5 (6)
C9—N2—C10—C11	−109.9 (8)	C29—N6—C30—C31	−130.2 (7)
Cu2—N3—C11—C10	15.0 (8)	Cu1—N7—C31—C30	33.9 (7)
C12—N3—C11—C10	−166.2 (7)	C32—N7—C31—C30	−153.4 (7)
N2—C10—C11—N3	−47.0 (8)	N6—C30—C31—N7	−50.9 (8)
Cu2—N3—C12—C13	2.5 (11)	Cu1—N7—C32—C33	−7.3 (10)
C11—N3—C12—C13	−176.0 (7)	C31—N7—C32—C33	−179.0 (6)
N3—C12—C13—C14	173.5 (7)	N7—C32—C33—C34	166.8 (8)
C12—C13—C14—C15	−173.1 (6)	C32—C33—C34—C35	−176.4 (7)
C13—C14—C15—C16	35.4 (10)	C33—C34—C35—C36	28.6 (11)
C13—C14—C15—C20	−152.3 (7)	C33—C34—C35—C40	−153.6 (8)
C14—C15—C16—C17	174.1 (7)	C34—C35—C36—C37	−180.0 (8)
C20—C15—C16—C17	1.2 (10)	C40—C35—C36—C37	2.0 (11)
C15—C16—C17—C18	0.0 (11)	C35—C36—C37—C38	−1.3 (13)
C16—C17—C18—C19	−1.2 (12)	C36—C37—C38—C39	0.0 (14)
C17—C18—C19—C20	1.2 (11)	C37—C38—C39—C40	0.3 (13)
C14—C15—C20—N4	7.7 (11)	C34—C35—C40—N8	2.4 (11)
C14—C15—C20—C19	−173.6 (7)	C34—C35—C40—C39	−179.5 (7)
C16—C15—C20—N4	−179.9 (6)	C36—C35—C40—N8	−179.8 (6)
C16—C15—C20—C19	−1.2 (11)	C36—C35—C40—C39	−1.7 (11)
C18—C19—C20—N4	178.8 (7)	C38—C39—C40—N8	178.8 (7)
C18—C19—C20—C15	0.0 (11)	C38—C39—C40—C35	0.5 (12)
O4—N4—C20—C15	−151.6 (8)	O8—N8—C40—C35	−165.2 (7)
O4—N4—C20—C19	29.6 (10)	O8—N8—C40—C39	16.5 (10)
O5—N4—C20—C15	24.0 (11)	O9—N8—C40—C35	14.2 (10)
O5—N4—C20—C19	−154.8 (7)	O9—N8—C40—C39	−164.1 (7)

Symmetry code: (i) $-x, y, -z+1/2$.

Hydrogen-bond geometry ($\text{\AA}$, $^\circ$)

$D\cdots H\cdots A$	$D\cdots H$	$H\cdots A$	$D\cdots A$	$D\cdots H\cdots A$
O1—H1 $\cdots$ Cl2	0.84 (1)	2.76 (8)	3.027 (6)	100 (6)
C2—H2 $\cdots$ O8 ⁱⁱ	0.95	2.52	3.218 (10)	130
C4—H4 $\cdots$ Cl2 ⁱⁱⁱ	0.95	2.73	3.633 (9)	160
C7—H7 $\cdots$ O3	0.95	2.40	2.726 (11)	100
C8—H8 $\cdots$ O1	0.95	2.64	3.300 (9)	127
C9—H9 $\cdots$ Cl6	0.95	2.96	3.559 (9)	122
C10—H10B $\cdots$ O7 ^{iv}	0.99	2.51	3.219 (12)	129
C11—H11B $\cdots$ Cl3 ^v	0.99	2.59	3.544 (8)	162
C13—H13 $\cdots$ Cl3	0.95	2.97	3.502 (8)	116
C14—H14 $\cdots$ O5	0.95	2.40	2.761 (9)	102
C27—H27 $\cdots$ O7	0.95	2.38	2.754 (11)	103
C28—H28 $\cdots$ O1	0.95	2.51	3.290 (9)	140
C30—H30B $\cdots$ Cl2 ⁱⁱⁱ	0.99	2.93	3.579 (7)	124
C30—H30B $\cdots$ Cl3 ⁱⁱⁱ	0.99	2.77	3.546 (8)	136
C33—H33 $\cdots$ Cl1	0.95	2.95	3.584 (9)	125

C34—H34···O9	0.95	2.29	2.757 (10)	109
C41—H41A···Cl1	0.99	2.88	3.869 (11)	176
C41—H41B···Cl1 ^{vi}	0.99	2.65	3.558 (10)	153

Symmetry codes: (ii) $x-1/2, -y+3/2, z-1/2$; (iii) $-x+1/2, y+1/2, -z+1/2$; (iv) $x, -y+1, z+1/2$; (v) $-x+1/2, -y+1/2, -z+1$; (vi) $-x+1/2, -y+3/2, -z+1$.