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Poly[(μ_3-5-hydroxyisophthalato)[μ_2-1,1′-(1,4-phenylene)bis(1*H*-imidazole)]copper]

Hong-Hong Tao,* Yu-Han Chen, Ya-Sai Liu and Zhuo-Ga Deji

People's Hospital of Tibet Autonomic Region, Lasa 850000, People's Republic of China. *Correspondence e-mail: taohonghong01@163.com

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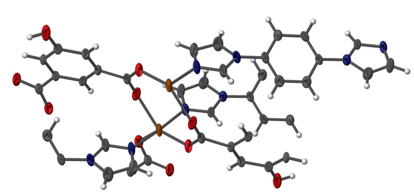
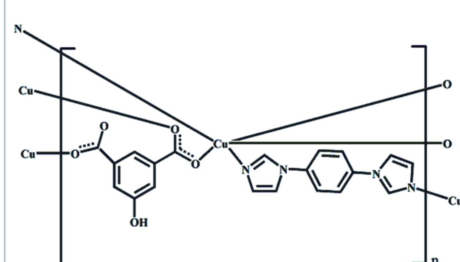
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $[Cu(C_8H_4O_5)(C_{12}H_{10}N_4)]_n$, was obtained by the reaction of copper(II) nitrate hydrate, with the OH-BDC organic linker and bib molecules [OH-BDC = 5-hydroxyisophthalic acid and bib = 1,4-bis(imidazol-1-yl)benzene]. The asymmetric unit comprises one Cu^{II} cation, one OH-BDC^{-2} dianion and a bib ligand. The Cu^{II} ion is coordinated by three carboxylate O atoms and two bib-N atoms, all from bridging ligands, to form a slightly distorted trigonal–bipyramidal geometry. The Cu^{II} ions are bridged by OH-BDC^{-2} ligands, forming a chain along the [100] direction; the chains are connected by bib molecules to form a two-dimensional net. In topological terms, considering the Cu^{II} atoms as nodes and the OH-BDC^{-2} ligands as linkers, the two-dimensional structure can be simplified as a typical 2-nodal 3,5 L2 plane network. The crystal structure features O—H$\cdots$O hydrogen bonds between OH-BDC^{-2} anions, resulting in a three-dimensional supramolecular network.

3D view



Chemical scheme



Structure description

A variety of metal–organic frameworks with intertesting structures have been reported based on 5-hydroxyisophthalic acid as this kind of carboxylate ligand offers six kinds of intricate connection models (Xu & Li, 2014). Supermolecules constructed by mixed ligands including carboxylate ligands and other N-donor molecules often show interesting networks compared with those compounds constructed by a single ligand (Xu *et al.*, 2015). However, there are only a few examples reported which are based on OH-BDC and bib molecules (Wang *et al.*, 2014; Liu & Guo., 2012; Su *et al.*, 2015; Li *et al.* 2015; Guo *et al.*, 2013). For this synthesis, we selected OH-BDC, bib organic ligands and copper(II) to construct a new supermolecule and present herein the structure of the title compound (Fig. 1), which is isostructural with the Mn^{II}-based analogue, (Li *et al.*, 2015).

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

D—H$\cdots$$A$	D—H	H$\cdots$$A$	$D$$\cdots$$A$	D—H$\cdots$$A$
O5—H5$\cdots$O4^{i}	0.82	1.84	2.660 (4)	177

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

The Cu^{II} ion is coordinated by three carboxylate O atoms and two bib-N atoms, all from bridging ligands, to form a slightly distorted trigonal–bipyramidal geometry. The Cu^{II} ions are bridged by OH-BDC^{-2} ligands, forming a chain along the [100] direction; the chains are connected by bib molecules to form a two-dimensional net. In topological terms, considering the Cu^{II} atoms as nodes and the OH-BDC^{-2} ligands as linkers, the two-dimensional structure can be simplified as a typical 2-nodal 3,5 L2 plane network.

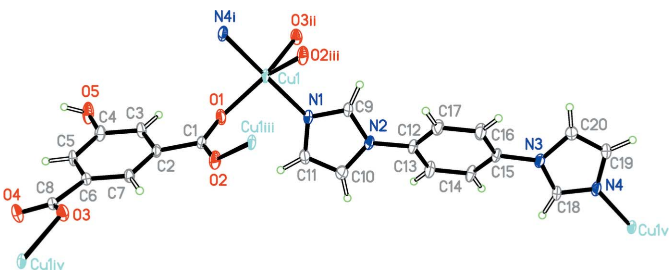


Figure 1
The asymmetric unit of the title compound, showing some symmetry-related atoms. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (i) $x-1, y+1, z-1$; (ii) $x+1, y, z$; (iii) $-x+1, -y+2, -z+1$; (iv) $x-1, y, z$; (v) $x+1, y-1, z+1$.]

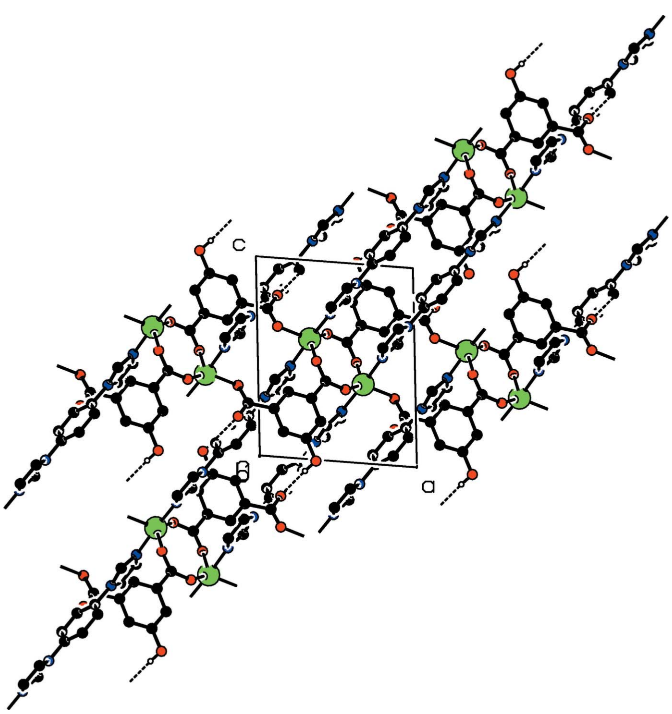


Figure 2
The crystal packing of the title complex, viewed along the b axis, with O—H hydrogen bonds shown as dashed lines.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Cu(C_8H_4O_5)(C_{12}H_{10}N_4)]$
M_r	453.89
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	296
a, b, c (Å)	9.948 (8), 9.955 (7), 12.043 (9)
α, β, γ (°)	66.38 (3), 82.99 (4), 61.08 (2)
V (Å^3)	952.6 (12)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.19
Crystal size (mm)	0.22 × 0.20 × 0.18
Data collection	
Diffractometer	Bruker *SMART* 1000 CCD
Absorption correction	Multi-scan (*SADABS*; Sheldrick, 2001)
T_{min}, T_{max}	0.853, 1
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10124, 4299, 3126
R_{int}	0.071
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.647
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.055, 0.130, 1.04
No. of reflections	4299
No. of parameters	272
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.46, −0.69

Computer programs: *SMART* and *SAINT-Plus* (Bruker, 2007), *SHELXL2014* (Sheldrick, 2015), *SHELXTL* (Sheldrick, 2008), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

The crystal structure features O—H$\cdots$O hydrogen bonds (Table 1) between OH-BDC^{-2} anions, resulting in a three-dimensional supramolecular network (Fig. 2).

Synthesis and crystallization

The title complex was synthesized by the reaction of 5-hydroxyisophthalic (9.1 mg, 0.05 mmol), 1,4-bis(1-imidazolyl)-benzene (10.5 mg, 0.05 mmol) in 8 ml of deionized water with copper(II) nitrate hydrate (24.1 mg, 0.1 mmol) in 20 ml of methanol and the mixture was refluxed for 0.5 h. To the above mixture, 0.5 ml of formic acid was added and the resulting fluid was placed in a Teflon-lined stainless-steel reactor. The reactor was heated to 413 K for 72 h. It was then cooled to room temperature. Blue block-shaped crystals were isolated in 68% yield (based on the OH-BDC ligand).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

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full crystallographic data

IUCrData (2016). **1**, x161802 [https://doi.org/10.1107/S2414314616018022]

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Poly[(μ_3-5-hydroxyisophthalato)[μ_2-1,1′-(1,4-phenylene)bis(1*H*-imidazole)]copper]

Crystal data

$[Cu(C_8H_4O_5)(C_{12}H_{10}N_4)]$	$Z = 2$
$M_r = 453.89$	$F(000) = 462$
Triclinic, $P\overline{1}$	$D_x = 1.582$ Mg m^{-3}
$a = 9.948$ (8) Å	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$b = 9.955$ (7) Å	Cell parameters from 2197 reflections
$c = 12.043$ (9) Å	$\theta = 2.3$–$27.5°$
$\alpha = 66.38$ (3)°	$\mu = 1.19$ mm^{-1}
$\beta = 82.99$ (4)°	$T = 296$ K
$\gamma = 61.08$ (2)°	Block, blue
$V = 952.6$ (12) Å^3	0.22 × 0.20 × 0.18 mm

Data collection

Bruker SMART 1000 CCD diffractometer	4299 independent reflections
Detector resolution: 13.6612 pixels mm^{-1}	3126 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.071$
Absorption correction: multi-scan (SADABS; Sheldrick, 2001)	$\theta_{max} = 27.4°$, $\theta_{min} = 1.9°$
$T_{min} = 0.853$, $T_{max} = 1$	$h = -12 \rightarrow 12$
10124 measured reflections	$k = -12 \rightarrow 12$
	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.055$	$w = 1/[\sigma^2(F_o^2) + (0.0495P)^2 + 0.2061P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.130$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.04$	$\Delta\rho_{max} = 0.46$ e Å^{-3}
4299 reflections	$\Delta\rho_{min} = -0.69$ e Å^{-3}
272 parameters	
0 restraints	

Special details

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

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

	x	y	z	U_{iso}*/U_{eq}
Cu1	0.66754 (5)	0.97776 (6)	0.39574 (4)	0.02984 (16)
O3	−0.1299 (3)	0.9861 (3)	0.3440 (2)	0.0344 (6)
O1	0.5542 (3)	0.8764 (3)	0.3623 (2)	0.0354 (6)
O2	0.3725 (3)	0.8802 (3)	0.4950 (2)	0.0392 (7)
O4	−0.1334 (3)	0.9181 (3)	0.1879 (2)	0.0406 (7)
O5	0.3567 (3)	0.9019 (4)	−0.0074 (2)	0.0511 (8)
H5	0.2856	0.9594	−0.0613	0.077*
N4	1.5339 (3)	0.1951 (4)	1.2624 (3)	0.0312 (7)
N3	1.3643 (3)	0.3795 (4)	1.1009 (3)	0.0291 (7)
N2	0.9579 (3)	0.6014 (4)	0.7009 (3)	0.0321 (7)
N1	0.7931 (3)	0.7678 (4)	0.5370 (3)	0.0355 (8)
C18	1.4343 (4)	0.2190 (4)	1.1838 (3)	0.0280 (8)
H18	1.4147	0.1361	1.1851	0.034*
C2	0.3368 (4)	0.8714 (4)	0.3064 (3)	0.0247 (7)
C8	−0.0688 (4)	0.9388 (4)	0.2585 (3)	0.0266 (8)
C3	0.3912 (4)	0.8762 (4)	0.1931 (3)	0.0299 (8)
H3	0.4888	0.8661	0.1775	0.036*
C4	0.2985 (4)	0.8964 (5)	0.1030 (3)	0.0308 (8)
C15	1.2612 (4)	0.4388 (4)	0.9979 (3)	0.0274 (8)
C1	0.4282 (4)	0.8745 (4)	0.3975 (3)	0.0263 (7)
C6	0.0964 (4)	0.9072 (4)	0.2403 (3)	0.0239 (7)
C7	0.1893 (4)	0.8869 (4)	0.3304 (3)	0.0248 (7)
H7	0.1534	0.8837	0.4059	0.030*
C5	0.1535 (4)	0.9073 (4)	0.1281 (3)	0.0286 (8)
H5A	0.0943	0.9148	0.0697	0.034*
C14	1.2764 (4)	0.3285 (5)	0.9494 (3)	0.0347 (9)
H14	1.3533	0.2179	0.9830	0.042*
C9	0.8926 (4)	0.7547 (5)	0.6102 (3)	0.0352 (9)
H9	0.9143	0.8397	0.6002	0.042*
C12	1.0637 (4)	0.5460 (4)	0.8018 (3)	0.0304 (8)
C19	1.5278 (4)	0.3485 (5)	1.2289 (3)	0.0404 (10)
H19	1.5854	0.3699	1.2684	0.048*
C13	1.1777 (4)	0.3812 (5)	0.8507 (3)	0.0381 (9)
H13	1.1882	0.3065	0.8182	0.046*
C20	1.4249 (5)	0.4632 (5)	1.1296 (3)	0.0394 (9)
H20	1.4001	0.5749	1.0890	0.047*
C16	1.1469 (5)	0.6036 (5)	0.9492 (3)	0.0412 (10)
H16	1.1364	0.6780	0.9820	0.049*
C17	1.0476 (5)	0.6568 (5)	0.8506 (4)	0.0417 (10)
H17	0.9703	0.7672	0.8176	0.050*
C10	0.8973 (5)	0.5107 (5)	0.6846 (4)	0.0459 (11)
H10	0.9208	0.4008	0.7328	0.055*
C11	0.7964 (5)	0.6151 (5)	0.5838 (4)	0.0443 (10)
H11	0.7380	0.5877	0.5509	0.053*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0259 (2)	0.0386 (3)	0.0216 (2)	−0.0161 (2)	−0.00973 (17)	−0.00445 (18)
O3	0.0231 (13)	0.0513 (16)	0.0316 (14)	−0.0191 (12)	0.0030 (11)	−0.0176 (12)
O1	0.0285 (14)	0.0472 (16)	0.0326 (14)	−0.0191 (13)	−0.0073 (11)	−0.0136 (12)
O2	0.0402 (15)	0.0571 (17)	0.0255 (14)	−0.0213 (14)	−0.0022 (12)	−0.0219 (12)
O4	0.0300 (14)	0.0565 (18)	0.0461 (17)	−0.0231 (14)	−0.0032 (12)	−0.0252 (14)
O5	0.0291 (15)	0.095 (2)	0.0294 (15)	−0.0217 (16)	0.0039 (12)	−0.0355 (16)
N4	0.0270 (16)	0.0384 (18)	0.0226 (15)	−0.0132 (14)	−0.0073 (12)	−0.0074 (13)
N3	0.0300 (16)	0.0303 (16)	0.0223 (15)	−0.0115 (14)	−0.0065 (12)	−0.0072 (12)
N2	0.0293 (16)	0.0287 (16)	0.0274 (16)	−0.0092 (14)	−0.0139 (13)	−0.0021 (13)
N1	0.0304 (17)	0.0398 (19)	0.0303 (17)	−0.0169 (15)	−0.0143 (13)	−0.0035 (14)
C18	0.0252 (18)	0.035 (2)	0.0220 (18)	−0.0112 (16)	−0.0049 (14)	−0.0120 (15)
C2	0.0236 (17)	0.0282 (18)	0.0225 (17)	−0.0115 (15)	−0.0050 (14)	−0.0093 (14)
C8	0.0243 (18)	0.0269 (18)	0.0274 (19)	−0.0137 (15)	−0.0050 (14)	−0.0056 (14)
C3	0.0180 (17)	0.042 (2)	0.0304 (19)	−0.0116 (16)	−0.0005 (14)	−0.0181 (16)
C4	0.0252 (18)	0.042 (2)	0.0240 (18)	−0.0108 (17)	−0.0002 (14)	−0.0172 (16)
C15	0.0213 (17)	0.0310 (19)	0.0203 (17)	−0.0071 (15)	−0.0061 (13)	−0.0060 (14)
C1	0.0257 (18)	0.0239 (17)	0.0240 (18)	−0.0099 (15)	−0.0092 (14)	−0.0039 (14)
C6	0.0211 (17)	0.0271 (18)	0.0243 (17)	−0.0121 (15)	−0.0028 (13)	−0.0087 (14)
C7	0.0254 (18)	0.0315 (18)	0.0203 (17)	−0.0137 (16)	0.0002 (13)	−0.0123 (14)
C5	0.0213 (17)	0.038 (2)	0.0278 (18)	−0.0105 (16)	−0.0061 (14)	−0.0167 (15)
C14	0.0271 (19)	0.032 (2)	0.0278 (19)	0.0009 (16)	−0.0112 (15)	−0.0108 (15)
C9	0.033 (2)	0.035 (2)	0.032 (2)	−0.0160 (18)	−0.0146 (16)	−0.0040 (16)
C12	0.0252 (18)	0.0308 (19)	0.0250 (19)	−0.0078 (16)	−0.0100 (14)	−0.0052 (15)
C19	0.045 (2)	0.050 (2)	0.031 (2)	−0.027 (2)	−0.0122 (17)	−0.0094 (18)
C13	0.038 (2)	0.036 (2)	0.032 (2)	−0.0065 (18)	−0.0131 (17)	−0.0140 (17)
C20	0.050 (2)	0.034 (2)	0.035 (2)	−0.022 (2)	−0.0095 (18)	−0.0083 (17)
C16	0.046 (2)	0.032 (2)	0.039 (2)	−0.0102 (19)	−0.0174 (18)	−0.0114 (17)
C17	0.046 (2)	0.0236 (19)	0.042 (2)	−0.0079 (18)	−0.0210 (19)	−0.0053 (17)
C10	0.054 (3)	0.034 (2)	0.044 (2)	−0.023 (2)	−0.019 (2)	−0.0016 (18)
C11	0.048 (3)	0.038 (2)	0.046 (2)	−0.023 (2)	−0.022 (2)	−0.0053 (18)

Geometric parameters (Å, º)

Cu1—N1	1.992 (3)	C2—C1	1.527 (4)
Cu1—N4^{i}	1.995 (3)	C8—C6	1.521 (5)
Cu1—O1	1.997 (3)	C3—C4	1.399 (5)
Cu1—O3^{ii}	2.066 (3)	C3—H3	0.9300
Cu1—O2^{iii}	2.170 (3)	C4—C5	1.397 (5)
O3—C8	1.269 (4)	C15—C14	1.379 (5)
O3—Cu1^{iv}	2.066 (3)	C15—C16	1.384 (5)
O1—C1	1.280 (4)	C6—C7	1.400 (4)
O2—C1	1.246 (4)	C6—C5	1.399 (5)
O2—Cu1^{iii}	2.170 (3)	C7—H7	0.9300
O4—C8	1.257 (4)	C5—H5A	0.9300
O5—C4	1.376 (4)	C14—C13	1.393 (5)

O5—H5	0.8200	C14—H14	0.9300
N4—C18	1.324 (4)	C9—H9	0.9300
N4—C19	1.387 (5)	C12—C13	1.384 (5)
N4—Cu1^{v}	1.995 (3)	C12—C17	1.384 (5)
N3—C18	1.360 (4)	C19—C20	1.363 (5)
N3—C20	1.394 (5)	C19—H19	0.9300
N3—C15	1.441 (4)	C13—H13	0.9300
N2—C9	1.351 (5)	C20—H20	0.9300
N2—C10	1.384 (5)	C16—C17	1.393 (5)
N2—C12	1.449 (4)	C16—H16	0.9300
N1—C9	1.331 (4)	C17—H17	0.9300
N1—C11	1.378 (5)	C10—C11	1.356 (5)
C18—H18	0.9300	C10—H10	0.9300
C2—C3	1.397 (5)	C11—H11	0.9300
C2—C7	1.405 (5)		

N1—Cu1—N4^{i}	176.06 (13)	C16—C15—N3	120.6 (3)
N1—Cu1—O1	91.42 (13)	O2—C1—O1	126.8 (3)
N4^{i}—Cu1—O1	89.73 (13)	O2—C1—C2	118.2 (3)
N1—Cu1—O3^{ii}	87.23 (13)	O1—C1—C2	115.0 (3)
N4^{i}—Cu1—O3^{ii}	94.62 (12)	C7—C6—C5	119.4 (3)
O1—Cu1—O3^{ii}	134.81 (11)	C7—C6—C8	121.6 (3)
N1—Cu1—O2^{iii}	89.72 (13)	C5—C6—C8	118.9 (3)
N4^{i}—Cu1—O2^{iii}	86.76 (13)	C6—C7—C2	119.9 (3)
O1—Cu1—O2^{iii}	133.92 (11)	C6—C7—H7	120.1
O3^{ii}—Cu1—O2^{iii}	91.26 (11)	C2—C7—H7	120.1
C8—O3—Cu1^{iv}	116.7 (2)	C4—C5—C6	120.7 (3)
C1—O1—Cu1	132.2 (2)	C4—C5—H5A	119.6
C1—O2—Cu1^{iii}	137.8 (2)	C6—C5—H5A	119.6
C4—O5—H5	109.5	C15—C14—C13	120.6 (3)
C18—N4—C19	105.6 (3)	C15—C14—H14	119.7
C18—N4—Cu1^{v}	125.6 (3)	C13—C14—H14	119.7
C19—N4—Cu1^{v}	128.7 (2)	N1—C9—N2	110.8 (3)
C18—N3—C20	106.4 (3)	N1—C9—H9	124.6
C18—N3—C15	124.3 (3)	N2—C9—H9	124.6
C20—N3—C15	128.9 (3)	C13—C12—C17	120.4 (3)
C9—N2—C10	107.5 (3)	C13—C12—N2	119.6 (3)
C9—N2—C12	126.1 (3)	C17—C12—N2	120.0 (3)
C10—N2—C12	126.2 (3)	C20—C19—N4	109.8 (3)
C9—N1—C11	105.7 (3)	C20—C19—H19	125.1
C9—N1—Cu1	122.9 (3)	N4—C19—H19	125.1
C11—N1—Cu1	131.3 (2)	C12—C13—C14	119.1 (3)
N4—C18—N3	111.9 (3)	C12—C13—H13	120.4
N4—C18—H18	124.1	C14—C13—H13	120.4
N3—C18—H18	124.1	C19—C20—N3	106.3 (3)
C3—C2—C7	120.3 (3)	C19—C20—H20	126.9
C3—C2—C1	119.5 (3)	N3—C20—H20	126.9
C7—C2—C1	119.6 (3)	C15—C16—C17	119.3 (4)

O4—C8—O3	125.7 (3)	C15—C16—H16	120.4
O4—C8—C6	118.0 (3)	C17—C16—H16	120.4
O3—C8—C6	116.3 (3)	C12—C17—C16	120.3 (3)
C2—C3—C4	119.9 (3)	C12—C17—H17	119.9
C2—C3—H3	120.1	C16—C17—H17	119.9
C4—C3—H3	120.1	C11—C10—N2	105.8 (3)
O5—C4—C5	122.6 (3)	C11—C10—H10	127.1
O5—C4—C3	117.7 (3)	N2—C10—H10	127.1
C5—C4—C3	119.7 (3)	C10—C11—N1	110.2 (3)
C14—C15—C16	120.3 (3)	C10—C11—H11	124.9
C14—C15—N3	119.1 (3)	N1—C11—H11	124.9

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5···O4^{vi}	0.82	1.84	2.660 (4)	177

Symmetry code: (vi) $-x, -y+2, -z$.