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Bis(2-hydroxybenzoato-kO)bis[3-(4methoxyphenyl)-4-(4-methylphenyl)-5- $(2-pyridyl)-4H-1,2,4-triazole-\kappa^2 N^1,N^5]$ copper(II) dihydrate

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Key indicators: single-crystal X-ray study; T = 296 K; mean σ (C–C) = 0.003 Å; R factor = 0.037; wR factor = 0.101; data-to-parameter ratio = 12.6.

In the title complex, $[Cu(C_7H_5O_3)_2(C_{21}H_{18}N_4O)_2]\cdot 2H_2O$, the Cu^{II} atom is located on a centre of inversion and exists in a tetragonally distorted octahedral geometry with a CuN₄O₂ chromophore. The intramolecular O-H···O hydrogen bond is highly strained due to the molecular geometry and, as a result, is much shorter than expected. Intermolecular C- $H \cdots O$ and $C - H \cdots O$ interactions are also observed.

Related literature

For general background to the coordination chemistry of 1,2,4-triazole derivatives, see: Koningsbruggen et al. (1997); Garcia et al. (1999); Klingele & Brooker (2003); Matsukizono et al. (2008); Suksrichavalit et al. (2009); Rubio et al. (2011). For their biological activity, see: Tozkoparan et al. (2000); Grénman et al. (2003); Alagarsamy et al. (2008); Isloor et al. (2009).



Experimental

Crystal data
$[Cu(C_7H_5O_3)_2(C_{21}H_{18}N_4O)_2]\cdot 2H_2O$
$M_r = 1058.58$
Triclinic, P1

a = 8.5933 (12) Å b = 10.6467 (15) Å c = 14.578 (2) Å

 $\alpha = 103.556 \ (2)^{\circ}$ $\beta = 91.501 \ (2)^{\circ}$ $\gamma = 101.843 \ (2)^{\circ}$ V = 1265.1 (3) Å³

T = 296 K $0.14 \times 0.13 \times 0.12 \text{ mm}$

Data collection

Z = 1

Bruker APEXII CCD	9025 measured reflections
diffractometer	4413 independent reflections
Absorption correction: multi-scan	3891 reflections with $I > 2\sigma(I)$
(SADABS; Sheldrick, 2003)	$R_{\rm int} = 0.024$
$T_{\min} = 0.933, T_{\max} = 0.942$	

Refinement

 $\begin{array}{l} R[F^2>2\sigma(F^2)]=0.037\\ wR(F^2)=0.101 \end{array}$ H atoms treated by a mixture of independent and constrained S = 1.08refinement $\Delta \rho_{\rm max} = 0.51$ e Å⁻³ 4413 reflections $\Delta \rho_{\rm min} = -0.33 \text{ e} \text{ Å}^{-3}$ 349 parameters

Table 1

Hydrogen-bond geometry (Å, °).

$D - H \cdots A$	D-H	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - H \cdots A$
$01W-H1F\cdots O2^{i}$	0.87 (4)	2.02 (4)	2.885 (3)	175 (4)
$01W-H1E\cdots O2$	0.78 (4)	2.08 (4)	2.865 (3)	174 (4)
$04-H4\cdots O3$	0.82	1.79	2.522 (3)	147

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

Data collection: APEX2 (Bruker, 2005); cell refinement: SAINT (Bruker, 2005); 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.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BR2165).

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Mo $K\alpha$ radiation $\mu = 0.50 \text{ mm}^{-3}$

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Bis(2-hydroxybenzoato- κO)bis[3-(4-methoxyphenyl)-4-(4-methylphenyl)-5-(2-pyridyl)-4H-1,2,4-triazole- $\kappa^2 N^1$, N^5]copper(II) dihydrate

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Comment

As the 1,2,4-triazole ring posesses strong electron donors, the coordination chemistry of 1,2,4-triazoles as a ligand is widely studied (Koningsbruggen *et al.*, 1997; Garcia *et al.*, 1999; Klingele & Brooker 2003; Matsukizono *et al.*, 2008; Suksrichavalit *et al.*, 2009; Rubio *et al.*, 2011). And some 1,2,4-triazole compounds have biological activities (Tozkoparan *et al.*, 2000; Grénman *et al.*, 2003; Alagarsamy *et al.*, 2008; Isloor *et al.*, 2009). We report here the crystal structure analysis of the title compound. The title copper(II) is surrounded by four N atoms [1.9774 (16)–2.0497 (16) Å] of the two 3-(4-methoxyphenyl)-4-(4-methylphenyl)-5-(2-pyridyl)-4*H*-1,2,4- triazoles in a plane, and two O atoms of the two carboxylate groups interact weakly at axial positions with the copper(II) atom at 2.4322 (16) Å.

There is an intramolecular hydrogen bond of O4-H4…O3, it is highly strained because of the fixed geometry of the molecule. As a result it is much shorter than would otherwise be expected for a bond with this angle.

Experimental

The title compound was prepared by reaction of 3-(4-methoxyphenyl)-4-(4-methylphenyl)-5-(2-pyridyl)-1,2,4-triazole with copper(II) salicylate in ethanol and water. To a warm solution of 0.684 grams of 3-(4-methoxyphenyl)-4-(4-methylphenyl)-5-(2-pyridyl)-1,2,4-triazole (2mmol) in 20 ml ethanol, 0.338 grams of copper(II) salicylate (1mmol) in 10 ml water was added. The filtrate was left to stand at room temperature for several days. The blue product was collected, and single crystals suitable for X-ray diffraction were selected.

Refinement

Positional parameters of all the H atoms were calculated geometrically and were allowed to ride on the C, N atoms to which they are bonded, riding with C—H = 0.93 Å (aromatic), 0.96 Å (methyl) or N—H = 0.85 Å, with Uĩso~(H) = 1.2 or 1.5 times U~eq~(C).

Figures



Fig. 1. The molecular structure of the title compound with the atomic labelling and the directions of the cell axes. Displacement ellipsoids are shown at 30% probability level.

Bis(2-hydroxybenzoato-κO)bis[3-(4-methoxyphenyl)-4-(4-methylphenyl)- 5-(2-pyridyl)-4H-1,2,4-triazole- $\kappa^2 N^1, N^5$]copper(II) dihydrate

Crystal data

 $[Cu(C_7H_5O_3)_2(C_{21}H_{18}N_4O)_2]$ ·2H₂O $M_r = 1058.58$ Triclinic, $P\overline{1}$ Hall symbol: -P 1 a = 8.5933 (12) Å *b* = 10.6467 (15) Å *c* = 14.578 (2) Å $\alpha = 103.556 \ (2)^{\circ}$ $\beta = 91.501 \ (2)^{\circ}$ $\gamma = 101.843 \ (2)^{\circ}$ V = 1265.1 (3) Å³

Data collection

Bruker APEXII CCD diffractometer	4413 independent reflections
Radiation source: fine-focus sealed tube	3891 reflections with $I > 2\sigma(I)$
graphite	$R_{\rm int} = 0.024$
ω scans	$\theta_{\text{max}} = 25.0^{\circ}, \ \theta_{\text{min}} = 1.4^{\circ}$
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	$h = -10 \rightarrow 10$
$T_{\min} = 0.933, T_{\max} = 0.942$	$k = -12 \rightarrow 12$
9025 measured reflections	$l = -17 \rightarrow 17$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.037$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.101$	H atoms treated by a mixture of independent and constrained refinement
<i>S</i> = 1.08	$w = 1/[\sigma^2(F_0^2) + (0.0507P)^2 + 0.3303P]$ where $P = (F_0^2 + 2F_c^2)/3$
4413 reflections	$(\Delta/\sigma)_{max} < 0.001$
349 parameters	$\Delta \rho_{max} = 0.51 \text{ e} \text{ Å}^{-3}$
0 restraints	$\Delta \rho_{\rm min} = -0.33 \text{ e} \text{ Å}^{-3}$

sup-2

Z = 1F(000) = 551 $D_{\rm x} = 1.389 {\rm Mg m}^{-3}$ Mo *K* α radiation, $\lambda = 0.71073$ Å Cell parameters from 9999 reflections $\theta = 2.4 - 25.7^{\circ}$ $\mu = 0.50 \text{ mm}^{-1}$ T = 296 KRhombic, blue $0.14 \times 0.13 \times 0.12 \text{ mm}$

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 (A^2)

	x	У	Z	$U_{\rm iso}*/U_{\rm eq}$
Cu1	0.0000	1.0000	1.0000	0.03718 (13)
N1	0.01756 (19)	0.84131 (16)	0.90177 (11)	0.0371 (4)
O3	0.10103 (18)	0.91416 (16)	1.12470 (12)	0.0527 (4)
N3	0.15216 (19)	0.73762 (16)	0.79657 (11)	0.0358 (4)
C8	0.2813 (2)	0.70780 (19)	0.73920 (13)	0.0352 (4)
N4	0.22652 (19)	1.06205 (16)	0.96344 (11)	0.0361 (4)
O2	-0.0191 (2)	0.70109 (16)	1.08112 (12)	0.0595 (4)
C10	0.4232 (3)	0.7231 (2)	0.60350 (15)	0.0441 (5)
H10	0.4341	0.7492	0.5470	0.053*
N2	-0.0804 (2)	0.72205 (16)	0.85894 (12)	0.0394 (4)
C2	0.0031 (2)	0.6597 (2)	0.79623 (14)	0.0374 (5)
C20	-0.1732 (3)	0.4437 (2)	0.77843 (15)	0.0444 (5)
H20	-0.1991	0.4751	0.8399	0.053*
01	-0.2764 (2)	0.14805 (16)	0.58065 (12)	0.0675 (5)
C13	0.3854 (3)	0.6414 (2)	0.76912 (15)	0.0434 (5)
H13	0.3714	0.6120	0.8242	0.052*
C22	0.0056 (3)	0.8111 (2)	1.13733 (16)	0.0449 (5)
C15	-0.0608 (2)	0.5241 (2)	0.73933 (14)	0.0390 (5)
C3	0.2794 (2)	0.97083 (19)	0.89747 (13)	0.0343 (4)
С9	0.2979 (3)	0.7490 (2)	0.65663 (15)	0.0415 (5)
Н9	0.2259	0.7936	0.6370	0.050*
C1	0.1555 (2)	0.85032 (19)	0.86417 (13)	0.0351 (4)
C12	0.5121 (3)	0.6189 (2)	0.71555 (16)	0.0503 (6)
H12	0.5848	0.5757	0.7361	0.060*
C23	-0.0796 (3)	0.8294 (2)	1.22638 (15)	0.0449 (5)
C6	0.4775 (3)	1.2099 (2)	0.97157 (16)	0.0483 (5)
H6	0.5423	1.2933	0.9965	0.058*
O4	0.0620 (3)	1.05550 (18)	1.28368 (14)	0.0759 (6)
H4	0.1018	1.0359	1.2332	0.114*
C16	-0.0206 (3)	0.4745 (2)	0.64802 (15)	0.0492 (5)
H16	0.0558	0.5268	0.6208	0.059*
C7	0.3238 (3)	1.1798 (2)	0.99837 (15)	0.0440 (5)
H7	0.2871	1.2438	1.0421	0.053*

C11	0.5333 (3)	0.6588 (2)	0.63257 (16)	0.0449 (5)
C4	0.4326 (2)	0.9949 (2)	0.86936 (15)	0.0439 (5)
H4A	0.4676	0.9305	0.8250	0.053*
C17	-0.0932 (3)	0.3490 (2)	0.59781 (16)	0.0543 (6)
H17	-0.0652	0.3164	0.5370	0.065*
C26	-0.2262 (5)	0.8563 (4)	1.3948 (2)	0.0911 (11)
H26	-0.2734	0.8640	1.4520	0.109*
C18	-0.2082 (3)	0.2706 (2)	0.63742 (16)	0.0486 (6)
C19	-0.2477 (3)	0.3182 (2)	0.72827 (16)	0.0477 (5)
H19	-0.3240	0.2658	0.7554	0.057*
C5	0.5333 (3)	1.1165 (2)	0.90825 (16)	0.0479 (5)
Н5	0.6377	1.1343	0.8914	0.058*
C25	-0.1175 (4)	0.9602 (3)	1.38054 (19)	0.0770 (9)
H25	-0.0921	1.0390	1.4273	0.092*
C14	0.6730 (3)	0.6345 (3)	0.5758 (2)	0.0704 (8)
H14A	0.6468	0.6308	0.5107	0.106*
H14B	0.6971	0.5520	0.5806	0.106*
H14C	0.7641	0.7051	0.5999	0.106*
C28	-0.1937 (3)	0.7267 (3)	1.24335 (19)	0.0616 (7)
H28	-0.2207	0.6470	1.1976	0.074*
C24	-0.0433 (3)	0.9495 (2)	1.29565 (17)	0.0553 (6)
C27	-0.2678 (4)	0.7400 (4)	1.3262 (2)	0.0855 (10)
H27	-0.3457	0.6705	1.3358	0.103*
C21	-0.3755 (4)	0.0575 (3)	0.6233 (2)	0.0760 (8)
H21A	-0.3161	0.0441	0.6756	0.114*
H21B	-0.4118	-0.0255	0.5776	0.114*
H21C	-0.4657	0.0925	0.6457	0.114*
O1W	0.1915 (2)	0.5712 (2)	0.96350 (16)	0.0732 (6)
H1F	0.145 (5)	0.488 (4)	0.949 (3)	0.110*
H1E	0.139 (5)	0.611 (4)	0.997 (3)	0.110*

Atomic displacement parameters $(Å^2)$

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0287 (2)	0.0316 (2)	0.0425 (2)	0.00245 (14)	0.01006 (14)	-0.00540 (14)
N1	0.0317 (9)	0.0324 (9)	0.0411 (9)	0.0041 (7)	0.0062 (7)	-0.0007 (7)
O3	0.0432 (9)	0.0530 (10)	0.0612 (10)	0.0065 (8)	0.0084 (7)	0.0154 (8)
N3	0.0334 (9)	0.0335 (9)	0.0365 (9)	0.0084 (7)	0.0071 (7)	-0.0004 (7)
C8	0.0343 (11)	0.0315 (10)	0.0358 (10)	0.0084 (8)	0.0057 (8)	-0.0012 (8)
N4	0.0301 (9)	0.0340 (9)	0.0387 (9)	0.0050 (7)	0.0063 (7)	-0.0003 (7)
O2	0.0772 (12)	0.0476 (10)	0.0523 (10)	0.0165 (9)	0.0166 (9)	0.0059 (8)
C10	0.0509 (13)	0.0424 (12)	0.0369 (11)	0.0074 (10)	0.0097 (9)	0.0072 (9)
N2	0.0352 (9)	0.0310 (9)	0.0440 (9)	0.0040 (7)	0.0061 (7)	-0.0039 (7)
C2	0.0359 (11)	0.0367 (11)	0.0369 (10)	0.0093 (9)	0.0028 (8)	0.0022 (9)
C20	0.0480 (13)	0.0402 (12)	0.0412 (11)	0.0122 (10)	0.0038 (10)	0.0001 (9)
01	0.0879 (14)	0.0356 (9)	0.0608 (11)	-0.0029 (9)	-0.0042 (9)	-0.0085 (8)
C13	0.0474 (13)	0.0474 (13)	0.0386 (11)	0.0174 (10)	0.0067 (9)	0.0103 (9)
C22	0.0436 (12)	0.0467 (13)	0.0473 (12)	0.0179 (11)	0.0044 (10)	0.0097 (10)

C15	0.0392 (11)	0.0346 (11)	0.0392 (11)	0.0105 (9)	0.0003 (9)	-0.0004 (9)
C3	0.0324 (10)	0.0351 (11)	0.0334 (10)	0.0084 (8)	0.0052 (8)	0.0033 (8)
C9	0.0442 (12)	0.0388 (12)	0.0428 (11)	0.0145 (10)	0.0033 (9)	0.0079 (9)
C1	0.0333 (11)	0.0344 (11)	0.0353 (10)	0.0097 (9)	0.0061 (8)	0.0018 (8)
C12	0.0464 (13)	0.0582 (15)	0.0534 (13)	0.0273 (11)	0.0085 (10)	0.0130 (11)
C23	0.0452 (13)	0.0469 (13)	0.0460 (12)	0.0195 (10)	0.0053 (10)	0.0097 (10)
C6	0.0369 (12)	0.0461 (13)	0.0499 (13)	-0.0046 (10)	0.0061 (10)	-0.0006 (10)
O4	0.1034 (17)	0.0521 (11)	0.0617 (12)	0.0080 (11)	-0.0054 (11)	0.0021 (9)
C16	0.0552 (14)	0.0407 (13)	0.0436 (12)	0.0049 (11)	0.0054 (10)	-0.0008 (10)
C7	0.0360 (11)	0.0392 (12)	0.0455 (12)	0.0016 (9)	0.0072 (9)	-0.0062 (9)
C11	0.0407 (12)	0.0425 (12)	0.0477 (12)	0.0100 (10)	0.0113 (9)	0.0020 (10)
C4	0.0363 (11)	0.0467 (13)	0.0461 (12)	0.0113 (10)	0.0129 (9)	0.0033 (10)
C17	0.0666 (16)	0.0466 (14)	0.0408 (12)	0.0103 (12)	0.0038 (11)	-0.0053 (10)
C26	0.123 (3)	0.103 (3)	0.074 (2)	0.065 (2)	0.052 (2)	0.036 (2)
C18	0.0582 (14)	0.0337 (12)	0.0475 (13)	0.0103 (10)	-0.0077 (11)	-0.0017 (9)
C19	0.0515 (14)	0.0364 (12)	0.0508 (13)	0.0048 (10)	0.0031 (10)	0.0060 (10)
C5	0.0304 (11)	0.0586 (14)	0.0489 (13)	0.0026 (10)	0.0098 (9)	0.0072 (11)
C25	0.121 (3)	0.072 (2)	0.0498 (15)	0.056 (2)	0.0108 (16)	0.0066 (14)
C14	0.0575 (17)	0.081 (2)	0.0727 (18)	0.0231 (15)	0.0279 (14)	0.0104 (15)
C28	0.0634 (16)	0.0577 (16)	0.0648 (16)	0.0147 (13)	0.0189 (13)	0.0144 (13)
C24	0.0698 (17)	0.0512 (15)	0.0499 (14)	0.0265 (13)	-0.0001 (12)	0.0112 (11)
C27	0.091 (2)	0.089 (2)	0.086 (2)	0.0244 (19)	0.0436 (19)	0.0328 (19)
C21	0.082 (2)	0.0402 (15)	0.090 (2)	-0.0022 (14)	0.0050 (17)	-0.0015 (14)
O1W	0.0569 (12)	0.0694 (13)	0.0760 (13)	-0.0073 (10)	0.0246 (10)	-0.0002 (11)

Geometric parameters (Å, °)

Cu1—N1	1.9773 (16)	C23—C24	1.402 (3)
Cu1—N4	2.0497 (16)	C6—C5	1.364 (3)
Cu1—O3	2.4322 (16)	C6—C7	1.383 (3)
N1—C1	1.314 (2)	С6—Н6	0.9300
N1—N2	1.368 (2)	O4—C24	1.344 (3)
O3—C22	1.282 (3)	O4—H4	0.8200
N3—C1	1.357 (2)	C16—C17	1.374 (3)
N3—C2	1.375 (3)	C16—H16	0.9300
N3—C8	1.449 (2)	С7—Н7	0.9300
C8—C13	1.369 (3)	C11—C14	1.508 (3)
C8—C9	1.376 (3)	C4—C5	1.384 (3)
N4—C7	1.334 (3)	C4—H4A	0.9300
N4—C3	1.357 (2)	C17—C18	1.387 (3)
O2—C22	1.236 (3)	C17—H17	0.9300
С10—С9	1.378 (3)	C26—C25	1.354 (5)
C10-C11	1.387 (3)	C26—C27	1.372 (5)
C10—H10	0.9300	C26—H26	0.9300
N2—C2	1.318 (3)	C18—C19	1.380 (3)
C2—C15	1.471 (3)	С19—Н19	0.9300
C20—C19	1.378 (3)	С5—Н5	0.9300
C20—C15	1.381 (3)	C25—C24	1.398 (4)
C20—H20	0.9300	С25—Н25	0.9300

01-C21 1.419 (3) $C14-H14B$ 0.9600 $C13-C12$ 1.384 (3) $C14-H14C$ 0.9600 $C13-H13$ 0.9300 $C28-C27$ 1.372 (4) $C22-C23$ 1.500 (3) $C28-C27$ 0.9300 $C15-C16$ 1.392 (3) $C27-H27$ 0.9300 $C3-C4$ 1.381 (3) $C21-H21A$ 0.9600 $C3-C1$ 1.461 (3) $C21-H21B$ 0.9600 $C2-C11$ 1.378 (3) $O1W-H1F$ 0.87 (4) $C12-C11$ 1.378 (3) $O1W-H1F$ 0.87 (4) $C12-C1-L1$ 0.9300 $O1W-H1F$ 0.87 (4) $C12-C1-L1$ 1.378 (3) $O1W-H1F$ 0.95 (7) $N1-Cu1-N4$ 80.33 (6) $C2-O4-H4$ 109.5 $N1-Cu1-O3$ 9.128 (6) $C17-C16-C15$ 120 (2) $O1-N1-Ca1$ 14.35 (13) $N-C-C-C6$ 122 09 (19) $N2=N1-Ca1$ 1.833 (13) $N-C-T-H7$ 19.0 $C1-N3-C2$ 105 25 (16) $C12-C11-C14$ 120 (2) $O2-O3-Ca1$ 112 82 (13) $C6-C7-H7$ 19.0 $C1-$	O1—C18	1.373 (3)	C14—H14A	0.9600
C13-C121384 (3)C14-H14C0.9600C13-H130.9300C28-C271.372 (4)C22-C231.500 (3)C28-H280.9300C15-C161.392 (3)C21-H210.9600C3-C41.381 (3)C21-H21A0.9600C3-C11.461 (3)C21-H21B0.9600C12-H120.930001W-H1F0.87 (4)C12-H120.930001W-H1F0.87 (4)C12-H120.930001W-H1F0.87 (4)C12-H120.930001W-H1F0.87 (4)C12-H120.930001W-H1F0.87 (4)C12-H120.930001W-H1F0.95 (5)N1-Cu1-O391.91 (6)C17-C16-C15120.4 (2)N1-Cu1-O391.91 (6)C17-C16-H161.98C1-N1-Cu1114.35 (13)N4-C7-C6122.09 (19)N2-N1-Cu1114.35 (13)N4-C7-H7119.0C2-O3-Cu1112.82 (13)C6-C7-H7119.0C2-N3-C2105.25 (16)C12-C11-C10118.0 (2)C1-N3-C2105.25 (16)C12-C11-C10118.0 (2)C1-N3-C3119.36 (18)C3-C4-C5118.87 (19)C13-C8-N3119.12 (17)C5-C4-H4A120.6C9-N3-C4118.56 (17)C16-C17-C18120.2 (2)C1-N3-C3119.36 (18)C3-C4-C5118.87 (19)C13-C2-N3119.13C3-C2-C4-D26119.5C1-N3-C111.75 (2)C2-C2-C4119.5C1-N3-C212.56 (14)C16-C17-H17119.2C1-N3-C3119	O1—C21	1.419 (3)	C14—H14B	0.9600
C13-H13 0.9300 C28-C27 1.372 (4) C22-C23 1.500 (3) C28-H28 0.9300 C3-C4 1.381 (3) C21-H21A 0.9300 C3-C4 1.381 (3) C21-H21A 0.9600 C3-C1 1.461 (3) C21-H21C 0.9600 C12-C11 1.378 (3) 01W-H1F 0.87 (4) C12-H12 0.9300 C21-H21C 0.9600 C23-C28 1.335 (3) N1-Cu1-M4 80.33 (6) C24-O4-H4 109.5 N1-Cu1-O3 91.91 (6) C17-C16-C15 129.4 (2) V4-Cu1-O3 91.28 (6) C17-C16-H16 119.8 C1-N1-Cu1 114.35 (13) N4-C7-H7 119.0 C22-O3-Cu1 112.82 (13) C6-C7-H7 119.0 C2-N3-C2 105.25 (16) C12-C11-C10 118.0 (2) C2-N3-C3 119.36 (18) C3-C4-C5 118.87 (19) C13-C8-C9 121.51 (19) C3-C4-C5 118.87 (19) C13-C8-N3 119.36 (18) C3-C4-H4A 120.6 C2-N3-C4 124.51 (16) C12-C11-C14 <td>C13—C12</td> <td>1.384 (3)</td> <td>C14—H14C</td> <td>0.9600</td>	C13—C12	1.384 (3)	C14—H14C	0.9600
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C13—H13	0.9300	C28—C27	1.372 (4)
C15-C16 1.392 ()C27-H27 0.9300 C3-C4 1.581 (3)C21-H21A 0.9600 C3-C1 1.461 (3)C21-H21B 0.9600 C9-H9 0.9300 C21-H21C 0.9600 C12-C11 1.378 (3) $0.W-H1F$ 0.78 (4)C12-H12 0.9300 $0.W-H1F$ 0.78 (4)C23-C28 1.385 (3) $W-H1F$ 0.78 (4)C12-H12 0.9300 $0.W-H1F$ 0.78 (4)C3-C28 1.385 (3) $W-H1F$ 0.78 (4)N1-Cu1-O3 91.91 (6) $C17-C16-C15$ 120.4 (2)N4-Cu1-O3 91.28 (6) $C17-C16-H16$ 119.8 C1-N1-Cu1 114.35 (13) $N4-C7-C6$ 122.09 (19)N2-N1-Cu1 16.33 (13) $N4-C7-C6$ 122.09 (19)C2-O3-Cu1 112.82 (13) $C6-C7-H7$ 119.0 C1-N3-C2 105.25 (16) $C12-C11-C14$ 120.9 (2)C1-N3-C3 126.29 (16) $C12-C11-C14$ 120.9 (2)C1-N3-C4 120.5 (16) $C10-C11-C14$ 120.9 (2)C1-N3-C5 119.5 (13) $C3-C4-C5$ 118.02 (12)C1-N4-C3 119.32 (13) $C3-C4-C5$ 118.91 (19)C1-N4-C3 119.32 (13) $C3-C4-C5$ 119.91 C1-N4-C4 120.69 (14) $C16-C17-H17$ 119.91 C1-N4-C3 119.52 (13) $C18-C17-H17$ 119.91 C1-N4-C4 120.69 (14) $C16-C17-H17$ 119.92 (12)C1-C4-H10 119.3 $C2-C2-C6-C27$ 119.57 (13)C1-N	C22—C23	1.500 (3)	C28—H28	0.9300
C3-C41.381 (a)C21-H21A0.9600C3-C11.461 (3)C21-H21B0.9600C3-C11.378 (3)O1W-H1F0.87 (4)C12-C111.378 (3)O1W-H1F0.87 (4)C12-H120.9300OIW-H1F0.87 (4)C12-H120.9300OIW-H1F0.87 (4)C23-C281.385 (3)IN1-Cu1-N480.33 (6)C24-O4-H14109.5N1-Cu1-N391.91 (6)C17-C16-C15120.4 (2)N4-Cu1-O391.28 (6)C17-C16-H16119.8C1-N1-Cu1114.35 (13)N4-C7-C6122.09 (19)N2-N1-Cu1136.33 (13)N4-C7-H7119.0C22-O3-Cu1112.82 (13)C6-C7-H7119.0C1-N3-C2105.25 (16)C12-C11-C10118.0 (2)C1-N3-C3126.29 (16)C12-C11-C14120.9 (2)C1-N3-C4126.29 (16)C12-C11-C14120.9 (2)C1-N3-C5118.87 (19)C3-C4-C5118.87 (19)C13-C8-N3119.36 (18)C3-C4-H4A120.6C9-C8-N3119.12 (17)C3-C4-H4A120.6C9-C8-N3119.32 (17)C16-C17-C18120.2 (2)C7-N4-Cu1126.69 (14)C16-C17-C18120.2 (2)C7-N4-Cu1126.69 (14)C16-C17-C18120.6C9-C10-C11121.3 (2)C25-C26-C27120.9 (3)C9-C10-C11123.2 (2)C25-C26-C27120.9 (3)C9-C10-C1119.3C25-C26-H26119.5 (2)C1-C10-H1019.3C26-C27-C2120.9 (3) <td>C15—C16</td> <td>1.392 (3)</td> <td>С27—Н27</td> <td>0.9300</td>	C15—C16	1.392 (3)	С27—Н27	0.9300
C3-C1 1.46 (3) C21-H21B 0.9600 C9-H9 0.9300 C21-H21C 0.9600 C12-C11 1.378 (3) OIW-H11F 0.75 (4) C12-C12 0.9300 OIW-H11E 0.78 (4) C23-C28 1.385 (3) V V N1-Cu1-03 91.91 (6) C17-C16-C15 120.4 (2) N4-Cu1-03 91.28 (6) C17-C16-H16 119.8 C1-N1-Cu1 114.35 (13) N4-C7-H7 119.0 C22-03-Cu1 112.82 (13) C6-C7-H7 119.0 C22-03-Cu1 112.82 (13) C6-C7-H7 119.0 C22-03-Cu1 112.82 (13) C1-C1-C14 120.9 (2) C1-N3-C2 105.25 (16) C12-C11-C10 118.80 (2) C1-N3-C8 126.29 (16) C12-C11-C14 120.9 (2) C3-N3-C8 128.45 (16) C10-C1-C14 120.1 (2) C3-C4-M3 119.36 (18) C3-C4-H4A 120.6 C7-N4-Cu1 126.69 (14) C16-C17-C18 120.9 (3) C9-C0-N3 119.36 (18) C3-C26-H26 119.5 C11-C10-H10 19.3	C3—C4	1.381 (3)	C21—H21A	0.9600
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C3—C1	1.461 (3)	C21—H21B	0.9600
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	С9—Н9	0.9300	C21—H21C	0.9600
C12—H12 0.9300 01W—H1E 0.78 (4) C23—C28 1.385 (3)	C12—C11	1.378 (3)	O1W—H1F	0.87 (4)
C23-C28 1,385 (3) NI-Cul-N4 80.33 (6) $C24-O4-H4$ 109.5 NI-Cul-O3 91.91 (6) $C17-C16-C15$ 120.4 (2) N4-Cul-O3 91.28 (6) $C17-C16-H16$ 119.8 C1-N1-N2 109.27 (16) $C15-C16-H16$ 119.8 C1-N1-Cul 114.35 (13) N4-C7-C6 122.09 (19) N2-N1-Cul 136.33 (13) N4-C7-H7 119.0 C22-03-Cul 122.23 (13) $C6-C7-H7$ 119.0 C1-N3-C2 105.25 (16) C12-C11-C10 118.0 (2) C1-N3-C8 126.29 (16) C12-C11-C14 120.9 (2) C2-N3-C8 128.45 (16) C10-C11-C14 121.1 (2) C13-C8-N3 119.36 (18) C3-C4-H4A 120.6 C9-C8-N3 119.12 (17) C5-C4-H4A 120.6 C9-C8-N3 119.12 (17) C5-C4-C7 120.9 (3) C9-C10-C11 126.69 (14) C16-C17-C18 120.2 (2) C7-N4-Cu1 166.69 (14) C16-C17-H17 119.9 C3-N4-Cu1 114.75 (13) C18-C17-H17 119.5 C11-C10-H10 19	C12—H12	0.9300	O1W—H1E	0.78 (4)
N1-Cu1-N480.33 (6)C24-O4-H4109.5N1-Cu1-O391.91 (6)C17-C16-C15120.4 (2)N4-Cu1-O391.28 (6)C17-C16-H16119.8C1-N1-N2109.27 (16)C15-C16-H16119.8C1-N1-Cu1114.35 (13)N4-C7-C6122.09 (19)N2-N1-Cu1128.21 (3)C6-C7-H7119.0C2-O3-Cu1128.22 (16)C12-C11-C10118.0 (2)C1-N3-C2105.25 (16)C12-C11-C14120.9 (2)C2-N3-C8126.29 (16)C12-C11-C14121.1 (2)C13-C8-C9121.51 (19)C3-C4-C5118.87 (19)C13-C8-N3119.36 (18)C3-C4-H4A120.6C9-C8-N3119.12 (17)C5-C4-H4A120.6C9-C8-N3119.12 (17)C5-C4-H4A120.6C9-C10-C11121.3 (2)C25-C26-C27120.9 (3)C9-C10-C11121.3 (2)C25-C26-C27120.9 (3)C9-C10-C1119.3C27-C26-H26119.5C1-C0-H10119.3C27-C26-H26119.5C1-C10-H10119.3C27-C26-H26119.5C1-C10-H10119.3C27-C26-H26119.5C1-C2-N310.19 (17)01-C18-C17119.8 (2)N3-C2-C15121.90 (19)C19-C19-C18120.2 (2)C15-C20-H20119.3C6-C5-H5120.4C8-C13-H13120.7C26-C25-C24120.2 (3)C19-C20-C15121.40 (2)C4-C5-H5120.4C8-C13-H13120.7C26-C25-H25119.9O2-C22-C23119.70 (2) </td <td>C23—C28</td> <td>1.385 (3)</td> <td></td> <td></td>	C23—C28	1.385 (3)		
N1-Cu1-O391.91 (6)C17-C16-C15120.4 (2)N4-Cu1-O391.28 (6)C17-C16-H16119.8C1-N1-N2109.27 (16)C15-C16-H16119.8C1-N1-Cu1114.35 (13)N4-C7-C6122.09 (19)N2-N1-Cu1136.33 (13)N4-C7-H7119.0C2-O3-Cu1112.82 (13)C6-C7-H7119.0C1-N3-C2105.25 (16)C12-C11-C10118.02 (2)C1-N3-C8126.29 (16)C12-C11-C14120.9 (2)C2-N3-C8128.45 (16)C10-C11-C14121.1 (2)C13-C8-C9121.51 (19)C3-C4-C5118.87 (19)C13-C8-N3119.36 (18)C3-C4-H4A120.6C9-C8-N3119.12 (17)C5-C4-H4A120.6C9-C8-N3119.12 (17)C16-C17-C18120.2 (2)C7-N4-Ca1126.69 (14)C16-C17-H17119.9C3-N4-Cu1114.75 (13)C18-C17-H17119.9C9-C10-C11121.3 (2)C25-C26-C27120.9 (3)C9-C10-H10119.3C27-C26-H26119.5C1-N2-N1106.23 (17)O1-C18-C17115.7 (2)N2-C2-C15121.90 (19)C19-C18-C17119.8 (2)N3-C2-C15121.90 (19)C19-C19-C18119.5 (2)C19-C20-C15121.4 (2)C20-C19-C18119.5 (2)C19-C20-C15121.4 (2)C20-C19-C18119.5 (2)C19-C20-C15121.4 (2)C20-C19-C18119.5 (2)C19-C20-C15121.4 (2)C20-C19-C18119.2 (2)C19-C20-C15121.6 (2)C14-C14-H14A <td>N1—Cu1—N4</td> <td>80.33 (6)</td> <td>C24—O4—H4</td> <td>109.5</td>	N1—Cu1—N4	80.33 (6)	C24—O4—H4	109.5
N4-Cu1-O391.28 (6)C17-C16-H16119.8C1-N1-N2109.27 (16)C15-C16-H16119.8C1-N1-Cu1114.35 (13)N4-C7-C6122.09 (19)N2-N1-Cu1136.33 (13)N4-C7-H7119.0C2-O3-Cu1112.82 (13)C6-C7-H7119.0C1-N3-C2105.25 (16)C12-C11-C14120.9 (2)C2-N3-C8126.29 (16)C10-C11-C14121.1 (2)C13-C8-C9121.51 (19)C3-C4-C5118.87 (19)C13-C8-N3119.36 (18)C3-C4-H4A120.6C7-N4-C3118.56 (17)C16-C17-C18120.2 (2)C7-N4-C41126.69 (14)C16-C17-H17119.9C3-N4-Cu1126.69 (14)C16-C17-H17119.9C3-N4-Cu1114.75 (13)C18-C17-H17119.9C9-C10-C11121.3 (2)C25-C26-C27120.9 (3)C9-C10-H10119.3C27-C26-H26119.5C1-N2-C15121.90 (19)C18-C17115.7 (2)N2-C2-N3110.19 (17)O1-C18-C17119.8 (2)C19-C20-C15121.90 (19)C19-C18-C17119.8 (2)C19-C20-C15121.40 (2)C20-C19-C18119.5 (2)C19-C20-C15121.40 (2)C20-C19-C18119.5 (2)C19-C20-C15121.40 (2)C20-C19-C18119.2 (2)C18-C13-H13120.7C26-C25-H25119.9O2-C22-C23119.7 (2)C4-C5-H15120.4C8-C13-H13120.7C26-C25-H25119.9O2-C22-C23119.7 (2)C11-C14-H14A109.5 <td>N1—Cu1—O3</td> <td>91.91 (6)</td> <td>C17—C16—C15</td> <td>120.4 (2)</td>	N1—Cu1—O3	91.91 (6)	C17—C16—C15	120.4 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	N4—Cu1—O3	91.28 (6)	C17—C16—H16	119.8
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C1—N1—N2	109.27 (16)	C15—C16—H16	119.8
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C1—N1—Cu1	114.35 (13)	N4—C7—C6	122.09 (19)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	N2—N1—Cu1	136.33 (13)	N4—C7—H7	119.0
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C22—O3—Cu1	112.82 (13)	С6—С7—Н7	119.0
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C1 - N3 - C2	105.25 (16)	C12—C11—C10	118.0 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C1—N3—C8	126.29 (16)	C12—C11—C14	120.9 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C2—N3—C8	128.45 (16)	C10—C11—C14	121.1 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C13—C8—C9	121.51 (19)	C3—C4—C5	118.87 (19)
C9-C8-N3119.12 (T)C5-C4-H4A120.6C7-N4-C3118.56 (17)C16-C17-C18120.2 (2)C7-N4-Cu1126.69 (14)C16-C17-H17119.9C3-N4-Cu1114.75 (13)C18-C17-H17119.9C9-C10-C11121.3 (2)C25-C26-C27120.9 (3)C9-C10-H10119.3C25-C26-H26119.5C11-C10-H10119.3C27-C26-H26119.5C2-N2-N1106.23 (17)O1-C18-C17115.7 (2)N2-C2-C15121.90 (19)C19-C18-C17119.8 (2)N3-C2-C15121.90 (19)C19-C18-C17119.5 (2)C19-C20-C15121.4 (2)C20-C19-H19120.2C19-C20-C15121.4 (2)C20-C19-H19120.2C19-C20-H20119.3C18-C19-H19120.2C15-C20-H20119.3C6-C5-C4119.2 (2)C18-O1-C21117.3 (2)C6-C5-H5120.4C8-C13-H13120.7C26-C25-C24120.2 (3)C12-C13-H13120.7C26-C25-H25119.9O2-C22-C33124.0 (2)C24-C25-H25119.9O2-C22-C23119.7 (2)C11-C14-H14B109.5O3-C22-C23116.2 (2)C11-C14-H14B109.5C20-C15-C2120.5 (18)C11-C14-H14C109.5C10-C15-C2120.3 (2)H14A-C14-H14C109.5C10-C15-C2120.3 (2)H14A-C14-H14C109.5C10-C15-C2120.2 (2)H14A-C14-H14C109.5C10-C15-C2120.10 (19)H14B-C14-H14C109.5	C13—C8—N3	119.36 (18)	C3—C4—H4A	120.6
C7-M4-C3118.56 (17)C16-C17-C18120.2 (2)C7-N4-Cu1126.69 (14)C16-C17-H17119.9C3-N4-Cu1114.75 (13)C18-C17-H17119.9C9-C10-C11121.3 (2)C25-C26-C27120.9 (3)C9-C10-H10119.3C25-C26-H26119.5C11-C10-H10119.3C27-C26-H26119.5C2-N2-N1106.23 (17)O1-C18-C19124.4 (2)N2-C2-N3110.19 (17)O1-C18-C17119.8 (2)N3-C2-C15121.90 (19)C19-C18-C17119.8 (2)C19-C20-C15121.4 (2)C20-C19-H19120.2C19-C20-C15121.4 (2)C20-C19-H19120.2C19-C20-H20119.3C18-C19-H19120.2C15-C20-H20119.3C18-C19-H19120.2C15-C20-H20119.3C6-C5-C4119.2 (2)C18-O1-C21117.3 (2)C6-C5-H5120.4C8-C13-H13120.7C26-C25-C24120.2 (3)C12-C13-H13120.7C26-C25-H25119.9O2-C22-C23119.7 (2)C11-C14-H14B109.5O3-C22-C23116.2 (2)C11-C14-H14B109.5C20-C15-C16118.57 (19)H14A-C14-H14B109.5C20-C15-C2120.5 (18)C11-C14-H14C109.5C20-C15-C2120.5 (18)C11-C14-H14C109.5C3-C2-C24120.70 (19)H14A-C14-H14C109.5	C9—C8—N3	119.12 (17)	С5—С4—Н4А	120.6
C7-M4-Cu1126.69 (14)C16-C17-H17119.9C3-M4-Cu1114.75 (13)C18-C17-H17119.9C9-C10-C11121.3 (2)C25-C26-C27120.9 (3)C9-C10-H10119.3C25-C26-H26119.5C11-C10-H10119.3C27-C26-H26119.5C2-N2-N1106.23 (17)O1-C18-C19124.4 (2)N2-C2-N3110.19 (17)O1-C18-C17115.7 (2)N2-C2-C15121.90 (19)C19-C18-C17119.8 (2)N3-C2-C15121.4 (2)C20-C19-C18119.5 (2)C19-C20-H20119.3C18-C19-H19120.2C15-C20-H20119.3C6-C5-C4119.2 (2)C18-C13-C12118.6 (2)C4-C5-H5120.4C8-C13-C12118.6 (2)C4-C5-H5120.4C8-C13-H13120.7C26-C25-C24120.2 (3)C12-C2-C23119.7 (2)C11-C14-H14B109.5C3-C22-C23116.2 (2)C11-C14-H14B109.5C20-C15-C16118.57 (19)H14A-C14-H14C109.5C16-C15-C2124.3 (2)H14A-C14-H14C109.5C4-C3-C4121.70 (19)H14B-C14-H14C109.5	C7—N4—C3	118.56 (17)	C16—C17—C18	120.2 (2)
C3-N4-Cu1114.75 (13) $C18-C17-H17$ 119.9 C9-C10-C11121.3 (2)C25-C26-C27120.9 (3)C9-C10-H10119.3C25-C26-H26119.5C11-C10-H10119.3C27-C26-H26119.5C2-N2-N1106.23 (17)O1-C18-C19124.4 (2)N2-C2-N3110.19 (17)O1-C18-C17115.7 (2)N2-C2-C15121.90 (19)C19-C18-C17119.8 (2)N3-C2-C15121.4 (2)C20-C19-C18119.5 (2)C19-C20-H20119.3C18-C19-H19120.2C15-C20-H20119.3C6-C5-C4119.2 (2)C18-C13-C12118.6 (2)C4-C5-H5120.4C8-C13-H13120.7C26-C25-C24120.2 (3)C12-C2-G3124.0 (2)C24-C25-H25119.9O2-C22-C23119.7 (2)C11-C14-H14B109.5C3-C20-C15-C16118.57 (19)H14A-C14-H14B109.5C20-C15-C2117.05 (18)C11-C14-H14C109.5C4-C5-C2-C4124.3 (2)H14A-C14-H14C109.5	C7—N4—Cu1	126.69 (14)	С16—С17—Н17	119.9
C9-C10-C11121.3 (2)C25-C26-C27120.9 (3)C9-C10-H10119.3C25-C26-H26119.5C11-C10-H10119.3C27-C26-H26119.5C2-N2-N1106.23 (17)O1-C18-C19124.4 (2)N2-C2-N3110.19 (17)O1-C18-C17115.7 (2)N2-C2-C15121.90 (19)C19-C18-C17119.8 (2)N3-C2-C15127.87 (18)C20-C19-C18119.5 (2)C19-C20-C15121.4 (2)C20-C19-H19120.2C19-C20-H20119.3C18-C19-H19120.2C15-C20-H20119.3C6-C5-C4119.2 (2)C18-O1-C21117.3 (2)C6-C5-H5120.4C8-C13-C12118.6 (2)C4-C5-H5120.4C8-C13-H13120.7C26-C25-C24120.2 (3)C12-C13-H13120.7C26-C25-H25119.9O2-C22-O3124.0 (2)C11-C14-H14A109.5O3-C22-C23119.7 (2)C11-C14-H14B109.5C20-C15-C16118.57 (19)H14A-C14-H14B109.5C20-C15-C2117.05 (18)C11-C14-H14C109.5C16-C15-C2124.3 (2)H14A-C14-H14C109.5N4-C3-C4121.70 (19)H14B-C14-H14C109.5	C3—N4—Cu1	114.75 (13)	С18—С17—Н17	119.9
C9-C10-H10119.3C25-C26-H26119.5C11-C10-H10119.3C27-C26-H26119.5C2-N2-N1106.23 (17)O1-C18-C19124.4 (2)N2-C2-N3110.19 (17)O1-C18-C17115.7 (2)N2-C2-C15121.90 (19)C19-C18-C17119.8 (2)N3-C2-C15127.87 (18)C20-C19-C18119.5 (2)C19-C20-H20119.3C18-C19-H19120.2C15-C20-H20119.3C6-C5-C4119.2 (2)C18-O1-C21117.3 (2)C6-C5-H5120.4C8-C13-C12118.6 (2)C4-C5-H5120.4C8-C13-H13120.7C26-C25-C24120.2 (3)C12-C13-H13120.7C26-C25-H25119.9O2-C22-O3124.0 (2)C24-C25-H25119.9O2-C22-C23119.7 (2)C11-C14-H14A109.5O3-C22-C23116.2 (2)C11-C14-H14B109.5C20-C15-C2117.05 (18)C11-C14-H14C109.5C16-C15-C2124.3 (2)H14A-C14-H14C109.5N4-C3-C4121.70 (19)H14B-C14-H14C109.5	C9—C10—C11	121.3 (2)	C25—C26—C27	120.9 (3)
C11—C10—H1019.3C27—C26—H2619.5C2—N2—N1106.23 (17)O1—C18—C19124.4 (2)N2—C2—N3110.19 (17)O1—C18—C17115.7 (2)N2—C2—C15121.90 (19)C19—C18—C17119.8 (2)N3—C2—C15127.87 (18)C20—C19—C18119.5 (2)C19—C20—C15121.4 (2)C20—C19—H19120.2C19—C20—H20119.3C18—C19—H19120.2C15—C20—H20119.3C6—C5—C4119.2 (2)C18—O1—C21117.3 (2)C6—C5—H5120.4C8—C13—C12118.6 (2)C4—C5—H5120.4C8—C13—H13120.7C26—C25—C24120.2 (3)C12—C13—H13120.7C26—C25—H25119.9O2—C22—O3124.0 (2)C14—C14—H14A109.5O3—C22—C23116.2 (2)C11—C14—H14B109.5C20—C15—C16118.57 (19)H14A—C14—H14B109.5C20—C15—C2117.05 (18)C11—C14—H14C109.5C16—C15—C2124.3 (2)H14A—C14—H14C109.5N4—C3—C4121.70 (19)H14B—C14—H14C109.5	C9—C10—H10	119.3	C25—C26—H26	119.5
C2N2N1106.23 (17)O1C18C19124.4 (2)N2C2N3110.19 (17)O1C18C17115.7 (2)N2C2C15121.90 (19)C19C18C17119.8 (2)N3C2C15127.87 (18)C20C19C18119.5 (2)C19C20C15121.4 (2)C20C19H19120.2C19C20H20119.3C18C19H19120.2C15C20H20119.3C6C5C4119.2 (2)C18O1C21117.3 (2)C6C5H5120.4C8C13C12118.6 (2)C4C5H5120.4C8C13H13120.7C26C25C24120.2 (3)C12C13H13120.7C26C25H25119.9O2C22O3124.0 (2)C11C14H14A109.5O3C22C23119.7 (2)C11C14H14B109.5C20C15C16118.57 (19)H14AC14H14B109.5C20C15C2117.05 (18)C11C14H14C109.5C16C15C2124.3 (2)H14AC14H14C109.5N4C3C4121.70 (19)H14BC14H14C109.5	С11—С10—Н10	119.3	С27—С26—Н26	119.5
N2-C2-N3 $110.19(17)$ O1-C18-C17 $115.7(2)$ N2-C2-C15 $121.90(19)$ C19-C18-C17 $119.8(2)$ N3-C2-C15 $127.87(18)$ C20-C19-C18 $119.5(2)$ C19-C20-C15 $121.4(2)$ C20-C19-H19 120.2 C19-C20-H20 119.3 C18-C19-H19 120.2 C15-C20-H20 119.3 C6-C5-C4 $119.2(2)$ C18-O1-C21 $117.3(2)$ C6-C5-H5 120.4 C8-C13-C12 $118.6(2)$ C4-C5-H5 120.4 C8-C13-H13 120.7 C26-C25-C24 $120.2(3)$ C12-C13-H13 120.7 C26-C25-H25 119.9 O2-C22-O3 $124.0(2)$ C11-C14-H14A 109.5 O3-C22-C23 $119.7(2)$ C11-C14-H14B 109.5 C20-C15-C16 $118.57(19)$ $H14A-C14-H14B$ 109.5 C20-C15-C2 $124.3(2)$ $H14A-C14-H14C$ 109.5 C16-C15-C2 $124.3(2)$ $H14A-C14-H14C$ 109.5 N4-C3-C4 $121.70(19)$ $H14B-C14-H14C$ 109.5	C2—N2—N1	106.23 (17)	O1—C18—C19	124.4 (2)
N2-C2-C15121.90 (19)C19-C18-C17119.8 (2)N3-C2-C15127.87 (18)C20-C19-C18119.5 (2)C19-C20-C15121.4 (2)C20-C19-H19120.2C19-C20-H20119.3C18-C19-H19120.2C15-C20-H20119.3C6-C5-C4119.2 (2)C18-O1-C21117.3 (2)C6-C5-H5120.4C8-C13-C12118.6 (2)C4-C5-H5120.4C8-C13-H13120.7C26-C25-C24120.2 (3)C12-C13-H13120.7C26-C25-H25119.9O2-C22-O3124.0 (2)C11-C14-H14A109.5O3-C22-C23116.2 (2)C11-C14-H14B109.5C20-C15-C16118.57 (19)H14A-C14-H14B109.5C20-C15-C2117.05 (18)C11-C14-H14C109.5C16-C15-C2124.3 (2)H14A-C14-H14C109.5N4-C3-C4121.70 (19)H14B-C14-H14C109.5	N2—C2—N3	110.19 (17)	O1—C18—C17	115.7 (2)
N3-C2-C15 $127.87 (18)$ $C20-C19-C18$ $119.5 (2)$ C19-C20-C15 $121.4 (2)$ $C20-C19-H19$ 120.2 C19-C20-H20 119.3 $C18-C19-H19$ 120.2 C15-C20-H20 119.3 $C6-C5-C4$ $119.2 (2)$ C18-O1-C21 $117.3 (2)$ $C6-C5-H5$ 120.4 C8-C13-C12 $118.6 (2)$ $C4-C5-H5$ 120.4 C8-C13-H13 120.7 $C26-C25-C24$ $120.2 (3)$ C12-C13-H13 120.7 $C26-C25-H25$ 119.9 O2-C22-O3 $124.0 (2)$ $C11-C14-H14A$ 109.5 O3-C22-C23 $119.7 (2)$ $C11-C14-H14B$ 109.5 C20-C15-C16 $118.57 (19)$ $H14A-C14-H14B$ 109.5 C20-C15-C2 $124.3 (2)$ $H14A-C14-H14C$ 109.5 C16-C15-C2 $124.3 (2)$ $H14A-C14-H14C$ 109.5 N4-C3-C4 $121.70 (19)$ $H14B-C14-H14C$ 109.5	N2—C2—C15	121.90 (19)	C19—C18—C17	119.8 (2)
C19-C20-C15121.4 (2)C20-C19-H19120.2C19-C20-H20119.3C18-C19-H19120.2C15-C20-H20119.3C6-C5-C4119.2 (2)C18-O1-C21117.3 (2)C6-C5-H5120.4C8-C13-C12118.6 (2)C4-C5-H5120.4C8-C13-H13120.7C26-C25-C24120.2 (3)C12-C13-H13120.7C26-C25-H25119.9O2-C22-O3124.0 (2)C24-C25-H25119.9O2-C22-C23119.7 (2)C11-C14-H14A109.5O3-C22-C23116.2 (2)C11-C14-H14B109.5C20-C15-C16118.57 (19)H14A-C14-H14B109.5C16-C15-C2124.3 (2)H14A-C14-H14C109.5N4-C3-C4121.70 (19)H14B-C14-H14C109.5	N3—C2—C15	127.87 (18)	C20—C19—C18	119.5 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C19—C20—C15	121.4 (2)	С20—С19—Н19	120.2
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	С19—С20—Н20	119.3	C18—C19—H19	120.2
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C15—C20—H20	119.3	C6—C5—C4	119.2 (2)
C8—C13—C12118.6 (2)C4—C5—H5120.4C8—C13—H13120.7C26—C25—C24120.2 (3)C12—C13—H13120.7C26—C25—H25119.9O2—C22—O3124.0 (2)C24—C25—H25119.9O2—C22—C23119.7 (2)C11—C14—H14A109.5O3—C22—C23116.2 (2)C11—C14—H14B109.5C20—C15—C16118.57 (19)H14A—C14—H14B109.5C20—C15—C2117.05 (18)C11—C14—H14C109.5C16—C15—C2124.3 (2)H14A—C14—H14C109.5N4—C3—C4121.70 (19)H14B—C14—H14C109.5	C18—O1—C21	117.3 (2)	С6—С5—Н5	120.4
C8—C13—H13120.7C26—C25—C24120.2 (3)C12—C13—H13120.7C26—C25—H25119.9O2—C22—O3124.0 (2)C24—C25—H25119.9O2—C22—C23119.7 (2)C11—C14—H14A109.5O3—C22—C23116.2 (2)C11—C14—H14B109.5C20—C15—C16118.57 (19)H14A—C14—H14B109.5C20—C15—C2117.05 (18)C11—C14—H14C109.5C16—C15—C2124.3 (2)H14A—C14—H14C109.5N4—C3—C4121.70 (19)H14B—C14—H14C109.5	C8—C13—C12	118.6 (2)	С4—С5—Н5	120.4
C12—C13—H13120.7C26—C25—H25119.9O2—C22—O3124.0 (2)C24—C25—H25119.9O2—C22—C23119.7 (2)C11—C14—H14A109.5O3—C22—C23116.2 (2)C11—C14—H14B109.5C20—C15—C16118.57 (19)H14A—C14—H14B109.5C20—C15—C2117.05 (18)C11—C14—H14C109.5C16—C15—C2124.3 (2)H14A—C14—H14C109.5N4—C3—C4121.70 (19)H14B—C14—H14C109.5	C8—C13—H13	120.7	C26—C25—C24	120.2 (3)
O2-C22-O3124.0 (2)C24-C25-H25119.9O2-C22-C23119.7 (2)C11-C14-H14A109.5O3-C22-C23116.2 (2)C11-C14-H14B109.5C20-C15-C16118.57 (19)H14A-C14-H14B109.5C20-C15-C2117.05 (18)C11-C14-H14C109.5C16-C15-C2124.3 (2)H14A-C14-H14C109.5N4-C3-C4121.70 (19)H14B-C14-H14C109.5	С12—С13—Н13	120.7	С26—С25—Н25	119.9
O2-C22-C23119.7 (2)C11-C14-H14A109.5O3-C22-C23116.2 (2)C11-C14-H14B109.5C20-C15-C16118.57 (19)H14A-C14-H14B109.5C20-C15-C2117.05 (18)C11-C14-H14C109.5C16-C15-C2124.3 (2)H14A-C14-H14C109.5N4-C3-C4121.70 (19)H14B-C14-H14C109.5	O2—C22—O3	124.0 (2)	C24—C25—H25	119.9
O3-C22-C23116.2 (2)C11-C14-H14B109.5C20-C15-C16118.57 (19)H14A-C14-H14B109.5C20-C15-C2117.05 (18)C11-C14-H14C109.5C16-C15-C2124.3 (2)H14A-C14-H14C109.5N4-C3-C4121.70 (19)H14B-C14-H14C109.5	O2—C22—C23	119.7 (2)	C11—C14—H14A	109.5
C20—C15—C16118.57 (19)H14A—C14—H14B109.5C20—C15—C2117.05 (18)C11—C14—H14C109.5C16—C15—C2124.3 (2)H14A—C14—H14C109.5N4—C3—C4121.70 (19)H14B—C14—H14C109.5	O3—C22—C23	116.2 (2)	C11—C14—H14B	109.5
C20—C15—C2117.05 (18)C11—C14—H14C109.5C16—C15—C2124.3 (2)H14A—C14—H14C109.5N4—C3—C4121.70 (19)H14B—C14—H14C109.5	C20—C15—C16	118.57 (19)	H14A—C14—H14B	109.5
C16—C15—C2124.3 (2)H14A—C14—H14C109.5N4—C3—C4121.70 (19)H14B—C14—H14C109.5	C20—C15—C2	117.05 (18)	C11—C14—H14C	109.5
N4—C3—C4 121.70 (19) H14B—C14—H14C 109.5	C16—C15—C2	124.3 (2)	H14A—C14—H14C	109.5
	N4—C3—C4	121.70 (19)	H14B—C14—H14C	109.5

111.19 (17)	C27—C28—C23	121.4 (3)
127.11 (18)	С27—С28—Н28	119.3
118.85 (19)	C23—C28—H28	119.3
120.6	O4—C24—C25	118.4 (3)
120.6	O4—C24—C23	122.1 (2)
109.03 (17)	C25—C24—C23	119.5 (3)
119.30 (17)	C28—C27—C26	119.6 (3)
131.67 (17)	С28—С27—Н27	120.2
121.7 (2)	С26—С27—Н27	120.2
119.1	O1—C21—H21A	109.5
119.1	O1—C21—H21B	109.5
118.2 (2)	H21A—C21—H21B	109.5
120.7 (2)	O1—C21—H21C	109.5
121.1 (2)	H21A—C21—H21C	109.5
119.5 (2)	H21B-C21-H21C	109.5
120.3	H1F—O1W—H1E	109 (4)
120.3		
	111.19 (17) 127.11 (18) 118.85 (19) 120.6 120.6 109.03 (17) 119.30 (17) 131.67 (17) 121.7 (2) 119.1 119.1 118.2 (2) 120.7 (2) 121.1 (2) 119.5 (2) 120.3 120.3	111.19(17)C27—C28—C23 $127.11(18)$ C27—C28—H28 $118.85(19)$ C23—C28—H28 120.6 O4—C24—C25 120.6 O4—C24—C23 $109.03(17)$ C25—C24—C23 $119.30(17)$ C28—C27—C26 $131.67(17)$ C28—C27—H27 $121.7(2)$ C26—C27—H27 119.1 O1—C21—H21A 119.2 H21A—C21—H21B $118.2(2)$ H21A—C21—H21B $120.7(2)$ O1—C21—H21C $121.1(2)$ H21A—C21—H21C $119.5(2)$ H21B—C21—H21C 120.3 H1F—O1W—H1E 120.3 H1F—O1W—H1E

Hydrogen-bond geometry (Å, °)

D—H···A	<i>D</i> —Н	H···A	$D \cdots A$	$D -\!\!\!-\!\!\!-\!\!\!\!-\!\!\!\!\!-\!\!\!\!\!-\!\!\!\!\!\!\!\!\!\!\!$
O1W—H1F···O2 ⁱ	0.87 (4)	2.02 (4)	2.885 (3)	175 (4)
O1W—H1E···O2	0.78 (4)	2.08 (4)	2.865 (3)	174 (4)
O4—H4…O3	0.82	1.79	2.522 (3)	147
Symmetry codes: (i) $-x$, $-y+1$, $-z+2$.				



