6973 measured reflections

 $R_{\rm int} = 0.024$

4652 independent reflections

3642 reflections with $I > 2\sigma(I)$

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(1,2-Disalicyloylhydrazine)hexakis-(pyridine)dinickel(II) 1,2-disalicyloylhydrazine solvate

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Key indicators: single-crystal X-ray study; T = 298 K; mean σ (C–C) = 0.005 Å; R factor = 0.035; wR factor = 0.102; data-to-parameter ratio = 13.2.

The title compound, $[Ni_2(C_{14}H_8N_2O_4)(C_5H_5N)_6]C_{14}H_{12}N_2O_4$, is composed of the complex $[Ni_2(C_{14}H_8N_2O_4)(C_5H_5N)_6]$ and a free ligand. Each nickel(II) coordination environment in the complex exhibits a distorted octahedral geometry. The dinuclear complex is centrosymmetric. The complex molecules are linked into one-dimensional chains via intermolecular O- $H \cdots O$ hydrogen bonds.

Related literature

The complex $[Ni_2(C_{14}H_8N_2O_4)(C_5H_5N)_6] \cdot 2C_5H_5N$ with 1,2disalicyloylhydrazine was reported previously (Chen & Liu, 2005). In that complex, the salicyloylhydrazine ligand functions as a tetranionic hexadentate ligand.



Experimental

Crystal data

$Ni_2(C_{14}H_8N_2O_4)(C_5H_5N)_6]$	$\beta = 85.285 \ (4)^{\circ}$
$C_{14}H_{12}N_2O_4$	$\gamma = 82.876 \ (4)^{\circ}$
$M_r = 1132.50$	$V = 1344.7 (9) \text{ Å}^3$
Friclinic, P1	Z = 1
a = 10.615 (4) Å	Mo $K\alpha$ radiation
p = 11.097 (4) Å	$\mu = 0.77 \text{ mm}^{-1}$
x = 12.094 (5) Å	T = 298 (2) K
$\alpha = 72.230 \ (4)^{\circ}$	$0.63 \times 0.52 \times 0.40 \text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer Absorption correction: multi-scan (SADABS: Sheldrick, 1996) $T_{\min} = 0.644, T_{\max} = 0.749$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.035$	352 parameters
$wR(F^2) = 0.102$	H-atom parameters constrained
S = 1.00	$\Delta \rho_{\rm max} = 0.40 \ {\rm e} \ {\rm \AA}^{-3}$
4652 reflections	$\Delta \rho_{\rm min} = -0.28 \text{ e } \text{\AA}^{-3}$

Table 1

Selected bond angles (°).

N1 ⁱ -Ni1-O2 ⁱ	90.10 (8)	O1-Ni1-N2	93.90 (9)
N1 ⁱ -Ni1-O1	79.56 (8)	N3-Ni1-N2	90.50 (9)
O2 ⁱ -Ni1-O1	169.66 (7)	N1 ⁱ -Ni1-N4	89.88 (8)
N1 ⁱ -Ni1-N3	169.09 (8)	O2 ⁱ -Ni1-N4	89.64 (8)
O2 ⁱ -Ni1-N3	100.36 (8)	O1-Ni1-N4	90.12 (9)
O1-Ni1-N3	89.96 (8)	N3-Ni1-N4	87.12 (9)
N1 ⁱ -Ni1-N2	93.18 (8)	N2-Ni1-N4	175.33 (8)
O2 ⁱ -Ni1-N2	86.83 (8)		

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

Table 2 Hydrogen-bond geometry (Å, °).

$D - H \cdots A$	D-H	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - \mathbf{H} \cdot \cdot \cdot A$
O4−H4···O2 ⁱⁱ	0.82	1.72	2.534 (3)	171
Symmetry code: (ii)	r v = 1 z + 1			

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); 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: KJ2063).

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(1,2-Disalicyloylhydrazine)hexakis(pyridine)dinickel(II) 1,2-disalicyloylhydrazine solvate

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Comment

A large number of salicylhydrazine complexes have been prepared and studied. However, research on the complex with 1,2-disalicyloylhydrazine is limited to only one complex $[Ni_2(C_{14}H_8N_2O_4)(C_5H_5N)_6]2C_5H_5N$ (Chen & Liu, 2005). We have synthesized another new complex $[Ni_2(C_{14}H_8N_2O_4)(C_5H_5N)_6]C_{14}H_{12}N_2O_4$, which has been characterized by X-ray diffraction and elemental analysis. Here we present the crystal structure of the title complex.

The title compound consists of the complex $[Ni_2(C_{14}H_8N_2O_4)(C_5H_5N)_6]$ and a free ligand (1,2-disalicyloylhydrazine) (Fig. 1). The Ni complex is formed by one chelated ligand, two nickel ions and six pyridine molecules. The ligand is present as the tetranionic hexadentate ligand dsh^{4–} and is linked with two nickel atoms. Both the binuclear nickel complex and the free ligand exhibit crystallographic centrosymmetry. From the data shown in Table 1, we can see that each nickel ion resides in a slightly distorted octahedral coordination environment, consisting of three pyridine N, a phenolate O, a carbonyl O and a hydrazine N of the ligand. which construct the fused five-membered and six-membered rings with each nickel atom. The two unique chelate rings, one five-membered and one six-membered, are near to coplanar with an 3.9 (3) ° dihedral angle.

As illustrated in Fig 2, the alternation of complex and free ligand molecules is linked into one-dimensional chain by intermolecular O4—H4 \cdots O2 H-bonds (Table 2) along the [1 – 1 1] axis.

Experimental

A solution of Ni(OAc)₂H₂O (0.0996 g, 0.4 mmol) in methanol (10 ml) was added to 1,2-disalicyloylhydrazine (0.054 g, 0.2 mmol) in pyridine (10 ml). After stirring the solution for four hours at room temperature, a reddish solution was obtained. After the solution had been standing for two weeks, red block crystals suitable for X-ray diffraction appeared. Yield: 0.086 g, 39%. m.p.> 573 K. Anal. for $C_{58}H_{50}N_{10}Ni_2O_8$: Calc. C, 61.46; H, 4.41; N, 11.36; Found: C, 61.42; H, 4.47; N, 11.33%.

Refinement

The H atoms on the ligands were allowed to ride on their parent atoms with $C(sp^2)$ —H distances of 0.93Å $[U_{iso}(H)=1.2U_{eq}(C)]$ and C(phenyl)—H distances of 0.93Å $[U_{iso}(H)=1.2U_{eq}(C)]$. The O—H distance is 0.820Å $[U_{iso}(H)=1.5U_{eq}(O)]$. All non-hydrogen atoms were refined anisotropically.

Figures



Fig. 1. The molecular structure of the title complex. Displacement ellipsoids are drawn at 30% probability level and H atoms have been omitted for clarity. symm. (A) -x + 1, -y + 2, -z, (B) -x, -y + 1, -z + 1

Fig. 2. Crystal packing of the title complex.

(1,2-Disalicyloylhydrazine)hexakis(pyridine)dinickel(II) 1,2-disalicyloylhydrazine solvate

Crystal data	
$[Ni_2(C_{14}H_8N_2O_4)(C_5H_5N)_6]\cdot C_{14}H_{12}N_2O_4$	Z = 1
$M_r = 1132.50$	$F_{000} = 588$
Triclinic, PT	$D_{\rm x} = 1.399 {\rm ~Mg~m}^{-3}$
<i>a</i> = 10.615 (4) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
b = 11.097 (4) Å	Cell parameters from 2995 reflections
c = 12.094 (5) Å	$\theta = 2.2 - 25.4^{\circ}$
$\alpha = 72.230 \ (4)^{\circ}$	$\mu = 0.77 \text{ mm}^{-1}$
$\beta = 85.285 \ (4)^{\circ}$	T = 298 (2) K
$\gamma = 82.876 \ (4)^{\circ}$	Block, red
$V = 1344.7 (9) \text{ Å}^3$	$0.63 \times 0.52 \times 0.40 \text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer	4652 independent reflections
Radiation source: fine-focus sealed tube	3642 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\rm int} = 0.024$
T = 298(2) K	$\theta_{\text{max}} = 25.0^{\circ}$
ϕ and ω scans	$\theta_{\min} = 1.8^{\circ}$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -12 \rightarrow 12$
$T_{\min} = 0.644, T_{\max} = 0.749$	$k = -9 \rightarrow 13$
6973 measured reflections	$l = -13 \rightarrow 14$

Refinement

Refinement on F^2

Secondary atom site location: difference Fourier map

Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.035$	H-atom parameters constrained
$wR(F^2) = 0.102$	$w = 1/[\sigma^2(F_o^2) + (0.048P)^2 + 0.4895P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.00	$(\Delta/\sigma)_{\rm max} = 0.001$
4652 reflections	$\Delta \rho_{\text{max}} = 0.40 \text{ e} \text{ Å}^{-3}$
352 parameters	$\Delta \rho_{\rm min} = -0.27 \ {\rm e} \ {\rm \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2 \operatorname{sigma}(F^2)$ 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.

	x	У	Ζ	$U_{\rm iso}*/U_{\rm eq}$
Ni1	0.58655 (3)	0.85566 (3)	0.16798 (3)	0.03193 (12)
N1	0.45229 (19)	1.05133 (19)	-0.00523 (17)	0.0279 (5)
N2	0.7511 (2)	0.9521 (2)	0.16127 (19)	0.0371 (5)
N3	0.5968 (2)	0.7776 (2)	0.34846 (18)	0.0381 (5)
N4	0.4278 (2)	0.7424 (2)	0.18095 (19)	0.0388 (5)
N5	0.0379 (3)	0.5115 (3)	0.5385 (2)	0.0567 (7)
Н5	0.0788	0.4495	0.5882	0.068*
01	0.46160 (17)	1.00370 (17)	0.19156 (14)	0.0366 (4)
O2	0.29489 (17)	1.27700 (16)	-0.11339 (15)	0.0358 (4)
O3	-0.0127 (2)	0.7197 (2)	0.4626 (2)	0.0711 (7)
O4	0.1637 (2)	0.43717 (19)	0.73076 (18)	0.0514 (5)
H4	0.2054	0.3913	0.7850	0.077*
C1	0.4151 (2)	1.0710 (2)	0.0945 (2)	0.0285 (6)
C2	0.3100 (2)	1.1727 (2)	0.0950 (2)	0.0306 (6)
C3	0.2541 (2)	1.2639 (2)	-0.0030 (2)	0.0327 (6)
C4	0.1496 (3)	1.3461 (3)	0.0180 (3)	0.0449 (7)
H4A	0.1106	1.4054	-0.0452	0.054*
C5	0.1028 (3)	1.3425 (3)	0.1281 (3)	0.0528 (8)
H5A	0.0329	1.3981	0.1381	0.063*
C6	0.1585 (3)	1.2572 (3)	0.2234 (3)	0.0506 (8)
Н6	0.1284	1.2558	0.2982	0.061*
C7	0.2595 (3)	1.1742 (3)	0.2060 (2)	0.0419 (7)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (A^2)

H7	0.2965	1.1159	0.2708	0.050*
C8	0.8504 (3)	0.8988 (3)	0.2266 (3)	0.0517 (8)
H8	0.8428	0.8217	0.2839	0.062*
С9	0.9626 (3)	0.9511 (3)	0.2139 (3)	0.0656 (10)
Н9	1.0285	0.9113	0.2627	0.079*
C10	0.9763 (3)	1.0626 (3)	0.1285 (3)	0.0642 (10)
H10	1.0528	1.0987	0.1157	0.077*
C11	0.8747 (3)	1.1202 (3)	0.0620 (3)	0.0642 (10)
H11	0.8801	1.1976	0.0046	0.077*
C12	0.7657 (3)	1.0625 (3)	0.0812 (3)	0.0488 (8)
H12	0.6974	1.1028	0.0355	0.059*
C13	0.5915 (3)	0.8589 (3)	0.4115 (3)	0.0541 (8)
H13	0.5839	0.9457	0.3730	0.065*
C14	0.5965 (4)	0.8199 (4)	0.5297 (3)	0.0730 (11)
H14	0.5928	0.8792	0.5704	0.088*
C15	0.6072 (4)	0.6928 (4)	0.5873 (3)	0.0803 (12)
H15	0.6117	0.6640	0.6677	0.096*
C16	0.6112 (4)	0.6085 (4)	0.5247 (3)	0.0689 (10)
H16	0.6187	0.5213	0.5619	0.083*
C17	0.6040 (3)	0.6544 (3)	0.4060 (3)	0.0485 (8)
H17	0.6042	0.5966	0.3642	0.058*
C18	0.3257 (3)	0.7548 (3)	0.2496 (3)	0.0502 (8)
H18	0.3233	0.8124	0.2920	0.060*
C19	0.2233 (3)	0.6862 (4)	0.2606 (3)	0.0644 (10)
H19	0.1534	0.6978	0.3094	0.077*
C20	0.2254 (4)	0.6018 (4)	0.2000 (4)	0.0723 (11)
H20	0.1574	0.5543	0.2065	0.087*
C21	0.3297 (4)	0.5875 (3)	0.1286 (3)	0.0666 (10)
H21	0.3337	0.5300	0.0861	0.080*
C22	0.4284 (3)	0.6599 (3)	0.1209 (3)	0.0499 (8)
H22	0.4984	0.6506	0.0716	0.060*
C23	0.0469 (3)	0.6322 (3)	0.5347 (3)	0.0493 (8)
C24	0.1349 (3)	0.6538 (3)	0.6131 (2)	0.0451 (7)
C25	0.1928 (3)	0.5585 (3)	0.7058 (3)	0.0442 (7)
C26	0.2772 (3)	0.5909 (3)	0.7717 (3)	0.0585 (9)
H26	0.3158	0.5283	0.8330	0.070*
C27	0.3040 (4)	0.7143 (4)	0.7470 (4)	0.0746 (11)
H27	0.3618	0.7347	0.7905	0.090*
C28	0.2452 (4)	0.8086 (4)	0.6577 (4)	0.0819 (12)
H28	0.2619	0.8926	0.6422	0.098*
C29	0.1627 (4)	0.7781 (3)	0.5924 (3)	0.0674 (10)
H29	0.1240	0.8422	0.5323	0.081*

Atomic displacement parameters (\AA^2)

	U^{11}	U ²²	U ³³	U^{12}	U^{13}	U^{23}
Ni1	0.0359 (2)	0.0282 (2)	0.02966 (19)	0.00429 (14)	-0.00713 (14)	-0.00721 (14)
N1	0.0280 (11)	0.0233 (11)	0.0314 (11)	0.0056 (8)	-0.0071 (9)	-0.0081 (9)

N2	0.0397 (13)	0.0301 (12)	0.0389 (12)	0.0012 (10)	-0.0122 (10)	-0.0058 (10)
N3	0.0445 (14)	0.0332 (13)	0.0328 (12)	-0.0011 (11)	-0.0077 (10)	-0.0040 (11)
N4	0.0379 (14)	0.0361 (13)	0.0397 (13)	-0.0001 (10)	-0.0056 (10)	-0.0076 (11)
N5	0.0685 (19)	0.0425 (15)	0.0532 (16)	0.0106 (14)	-0.0261 (13)	-0.0059 (13)
01	0.0453 (11)	0.0360 (10)	0.0267 (9)	0.0095 (8)	-0.0078 (8)	-0.0106 (8)
02	0.0401 (11)	0.0291 (10)	0.0345 (10)	0.0082 (8)	-0.0055 (8)	-0.0076 (8)
03	0.0887 (19)	0.0464 (14)	0.0629 (15)	0.0190 (13)	-0.0272 (13)	0.0024 (12)
O4	0.0591 (14)	0.0373 (12)	0.0513 (12)	0.0072 (10)	-0.0215 (10)	-0.0036 (10)
C1	0.0285 (14)	0.0281 (14)	0.0303 (14)	-0.0005 (11)	-0.0041 (11)	-0.0108 (11)
C2	0.0300 (14)	0.0292 (14)	0.0348 (14)	-0.0016 (11)	-0.0051 (11)	-0.0125 (11)
C3	0.0321 (14)	0.0283 (14)	0.0387 (15)	-0.0009 (11)	-0.0028 (11)	-0.0123 (12)
C4	0.0406 (17)	0.0380 (17)	0.0510 (18)	0.0116 (13)	-0.0040 (14)	-0.0115 (14)
C5	0.0441 (18)	0.0492 (19)	0.064 (2)	0.0144 (15)	0.0028 (15)	-0.0234 (17)
C6	0.0505 (19)	0.057 (2)	0.0478 (17)	0.0094 (16)	0.0045 (14)	-0.0284 (16)
C7	0.0441 (17)	0.0445 (17)	0.0385 (15)	0.0057 (14)	-0.0060 (13)	-0.0172 (14)
C8	0.0464 (19)	0.0376 (17)	0.063 (2)	-0.0010 (14)	-0.0196 (16)	-0.0007 (15)
C9	0.048 (2)	0.052 (2)	0.091 (3)	-0.0017 (17)	-0.0284 (19)	-0.007 (2)
C10	0.050 (2)	0.062 (2)	0.083 (3)	-0.0165 (18)	-0.0067 (18)	-0.020 (2)
C11	0.074 (3)	0.049 (2)	0.062 (2)	-0.0234 (19)	-0.0175 (19)	0.0038 (17)
C12	0.054 (2)	0.0391 (17)	0.0490 (18)	-0.0059 (15)	-0.0206 (15)	-0.0022 (15)
C13	0.077 (2)	0.0435 (18)	0.0432 (17)	0.0012 (16)	-0.0187 (16)	-0.0131 (15)
C14	0.105 (3)	0.075 (3)	0.0423 (19)	0.002 (2)	-0.0203 (19)	-0.0234 (19)
C15	0.100 (3)	0.096 (3)	0.0348 (18)	-0.010 (3)	-0.0134 (19)	-0.001 (2)
C16	0.081 (3)	0.054 (2)	0.054 (2)	-0.009 (2)	-0.0116 (19)	0.0109 (19)
C17	0.0482 (19)	0.0418 (18)	0.0493 (18)	-0.0016 (14)	-0.0078 (14)	-0.0041 (15)
C18	0.0499 (19)	0.0480 (19)	0.0465 (17)	0.0000 (15)	0.0034 (15)	-0.0081 (15)
C19	0.050 (2)	0.061 (2)	0.067 (2)	-0.0070 (18)	0.0094 (17)	0.0012 (19)
C20	0.056 (2)	0.057 (2)	0.095 (3)	-0.0221 (19)	-0.008 (2)	-0.002 (2)
C21	0.071 (3)	0.053 (2)	0.084 (3)	-0.0117 (19)	-0.018 (2)	-0.026 (2)
C22	0.0498 (19)	0.0480 (19)	0.0546 (18)	-0.0010 (15)	-0.0078 (15)	-0.0195 (16)
C23	0.056 (2)	0.0427 (18)	0.0397 (16)	0.0099 (15)	0.0018 (14)	-0.0052 (14)
C24	0.0491 (18)	0.0384 (17)	0.0428 (16)	0.0048 (14)	0.0024 (14)	-0.0096 (14)
C25	0.0435 (17)	0.0400 (17)	0.0458 (17)	0.0075 (14)	0.0005 (13)	-0.0130 (14)
C26	0.059 (2)	0.054 (2)	0.063 (2)	0.0058 (17)	-0.0104 (17)	-0.0201 (18)
C27	0.077 (3)	0.067 (3)	0.092 (3)	-0.008 (2)	-0.011 (2)	-0.040 (2)
C28	0.094 (3)	0.049 (2)	0.105 (3)	-0.015 (2)	-0.004 (3)	-0.023 (2)
C29	0.084 (3)	0.042 (2)	0.069 (2)	-0.0011 (18)	-0.002 (2)	-0.0088 (18)

Geometric parameters (Å, °)

Ni1—N1 ⁱ	1.974 (2)	C9—C10	1.364 (5)
Ni1—O2 ⁱ	2.0455 (18)	С9—Н9	0.9300
Ni1—O1	2.0549 (18)	C10—C11	1.370 (5)
Ni1—N3	2.095 (2)	C10—H10	0.9300
Ni1—N2	2.142 (2)	C11—C12	1.360 (4)
Ni1—N4	2.192 (2)	C11—H11	0.9300
N1—C1	1.312 (3)	C12—H12	0.9300
N1—N1 ⁱ	1.410 (4)	C13—C14	1.365 (4)

N2-Cl21.327 (3)Cl4-Cl51.365 (5)N2-C81.335 (4)Cl4-H140.9300N3-Cl71.328 (4)Cl5-Cl61.367 (5)N3-Cl31.341 (4)Cl5-H150.9300N4-Cl81.330 (4)Cl6-Cl71.374 (4)N4-C221.331 (4)Cl6-H160.9300N5-C231.341 (4)Cl7-H170.9300N5-N5"0.8600Cl8-H180.9300N5-H50.8600Cl8-H180.9300O1-Cl1.284 (3)Cl9-C201.352 (5)O2-Ni1 ⁱ 2.0455 (18)C20-C211.370 (5)O3-C231.356 (3)C21-C221.378 (4)O4-H40.8200C21-H210.9300C1-C21.485 (4)C22-H220.9300C2-C71.409 (4)C24-C291.389 (4)C2-C31.419 (4)C24-C291.389 (4)C2-C31.373 (4)C25-C261.370 (5)C5-C61.372 (4)C26-H260.9300C5-H5A0.9300C26-C271.370 (5)C5-C61.372 (4)C26-H260.9300C5-H5A0.9300C27-C281.382 (5)C6-C71.371 (4)C27-H270.9300C5-H5A0.9300C28-H280.9300C5-H5A0.9300C28-H280.9300C5-H5A0.9300C28-H280.9300C5-H5A0.9300C28-H280.9300C5-H5A0.9300C28-H280.9300C6-H60.9300C28-H280.9300
N2-C81.335 (4)C14-H140.9300N3-C171.328 (4)C15-C161.367 (5)N3-C131.341 (4)C15-H150.9300N4-C181.330 (4)C16-C171.374 (4)N4-C221.331 (4)C16-H160.9300N5-C231.341 (4)C17-H170.9300N5-M5 ⁱⁱ 1.378 (5)C18-C191.378 (5)O1-C11.284 (3)C19-C201.352 (5)O2-C31.339 (3)C19-H190.9300O2-Ni1 ⁱ 2.0455 (18)C20-C211.378 (4)O3-C231.255 (3)C20-H1200.9300O4-C251.356 (3)C21-H210.9300C1-C21.485 (4)C22-H220.9300C1-C21.485 (4)C22-H220.9300C1-C21.485 (4)C22-H220.9300C2-C71.409 (4)C23-C241.473 (4)C2-C31.419 (4)C24-C251.389 (4)C2-C41.373 (4)C24-C251.389 (4)C3-C41.409 (4)C24-C251.389 (4)C4-C51.373 (4)C26-C261.394 (4)C4-C51.373 (4)C26-C261.394 (4)C4-H4A0.9300C26-C271.380 (5)C5-C61.372 (4)C26-H260.9300C5-H5A0.9300C27-C281.382 (5)C6-C71.371 (4)C27-H270.9300C6-H60.9300C28-C291.362 (5)C7-H70.9300C28-H280.9300C8-H80.9300C28-C1
N3-C171.328 (4)C15-C161.367 (5)N3-C131.341 (4)C15-H150.9300N4-C181.330 (4)C16-C171.374 (4)N4-C221.331 (4)C17-H170.9300N5-C231.341 (4)C17-H170.9300N5-N5 ⁱⁱ 1.378 (5)C18-C191.378 (5)N5-H50.8600C18-H180.9300O1-C11.284 (3)C19-C201.352 (5)O2-C31.339 (3)C19-C100.9300O2-Ni1 ⁱ 2.0455 (18)C20-C211.378 (4)O4-H40.8200C21-H210.9300C4-C251.356 (3)C21-C221.378 (4)O4-H40.8200C21-H210.9300C2-C71.409 (4)C23-C241.473 (4)C2-C31.419 (4)C24-C291.389 (4)C3-C41.404 (4)C24-C251.394 (4)C4-C51.373 (4)C26-C261.394 (4)C4-C51.373 (4)C26-C271.389 (3)C5-C61.372 (4)C26-H260.9300C5-H5A0.9300C27-C281.382 (5)C6-H60.9300C28-C291.362 (5)C7-H70.9300C28-C291.362 (5)C7-H70.9300C28-H280.9300C6-H60.9300C28-H280.9300C5-H5A0.9300C28-H280.9300C6-H60.9300C28-H280.9300C6-H60.9300C28-H280.9300C7-H70.956 (8)C9-C10-H10120.8 </td
N3C131.341 (4)C15H150.9300N4C181.330 (4)C16C171.374 (4)N4C221.331 (4)C16H160.9300N5C231.341 (4)C17H170.9300N5N5 ⁱⁱ 1.378 (5)C18C191.378 (5)N5H50.8600C18H180.9300O1C11.284 (3)C19C201.352 (5)O2C31.339 (3)C19H190.9300O2Ni1 ⁱ 2.0455 (18)C20C211.378 (4)O4C251.356 (3)C21C221.378 (4)O4H40.8200C21H210.9300C1C21.485 (4)C22H220.9300C1C21.485 (4)C22C241.473 (4)C2C31.419 (4)C24C251.407 (4)C2C41.409 (4)C24C251.407 (4)C2C51.373 (4)C25C261.394 (40)C3C41.494 (4)C24C251.407 (4)C4C51.372 (4)C26H260.9300C5C61.372 (4)C26H260.9300C5C61.371 (4)C27H270.9300C6C71.371 (4)C27H270.9300C8C91.366 (4)C29H101.83 (3)N1 ¹ -N1-O2 ⁱ 90.300C28C291.362 (5)C7H70.9300C28C291.362 (5)C7H70.9300C28C191.362 (5)C7H70.9300C28C191.362 (5)C9D1169.66 (7)C11C10-H10 <td< td=""></td<>
N4—C18 1.330 (4) C16—C17 1.374 (4) N4—C22 1.331 (4) C16—H16 0.9300 N5—C23 1.341 (4) C17—H17 0.9300 N5—N5 ⁱⁱ 1.378 (5) C18—C19 1.378 (5) N5—H5 0.8600 C18—H18 0.9300 O1—C1 1.284 (3) C19—C20 1.352 (5) O2—C3 1.339 (3) C19—H19 0.9300 O2—Ni1 ⁱ 2.0455 (18) C20—C21 1.378 (4) O3—C23 1.235 (3) C21—H20 0.9300 O4—C45 1.356 (3) C21—H21 0.9300 C1—C2 1.485 (4) C22—H22 0.9300 C2—C7 1.485 (4) C24—C29 1.389 (4) C2—C3 1.419 (4) C24—C25 1.407 (4) C2—C3 1.419 (4) C24—C25 1.407 (4) C2—C5 1.371 (4) C26—C27 1.370 (5) C5—C6 1.372 (4) C26—C27 1.370 (5) C5—C4 1.371 (4) C27—H27 0.9300 C4—C5 1.371 (4) C27—H27 0.9300 C5—H5A 0.9300 C28—C29 1.362 (5) C6—C7 1.371 (4) C27—H27 0.9300 C8—C5 1.366 (7)<
N4C221.331 (4)C16H160.9300N5C231.341 (4)C17H170.9300N5NS ^{di} 1.378 (5)C18C191.378 (5)N5H50.8600C18H180.9300O1C11.284 (3)C19C201.352 (5)O2C31.339 (3)C19H190.9300O2Ni1 ¹ 2.0455 (18)C20C211.370 (5)O3C231.235 (3)C20-H200.9300O4C251.356 (3)C21C221.378 (4)O4H40.8200C21H210.9300C2C71.485 (4)C22-H220.9300C2C71.485 (4)C24C291.389 (4)C2C31.419 (4)C24C291.389 (4)C2C41.373 (4)C26C271.370 (5)C3C41.404 (4)C26C271.370 (5)C5C61.372 (4)C26-H260.9300C5C61.372 (4)C26-H260.9300C5H5A0.9300C27C281.382 (5)C6C71.371 (4)C27-H270.9300C5H60.9300C28-H280.9300C6H60.9300C28-H280.9300C8C91.366 (4)C29-H291.362 (5)C7H70.9300C28-H280.9300C8C91.366 (7)C11C10H10120.8N1 ¹ -N1-O17.956 (8)C9C10H10120.8N1 ¹ -N1-N3169.09 (8)C12C11H11120.5O2 ¹ -N1-N3100.36 (8)C12C11H11120.
NS-C231.341 (4)C17-H170.9300NS-N5 ⁱⁱ 1.378 (5)C18-C191.378 (5)N5-H50.8600C18-H180.9300O1-C11.284 (3)C19-C201.352 (5)02-C31.339 (3)C19-H190.930002-Nii ¹ 2.0455 (18)C20-C211.370 (5)03-C231.235 (3)C20-H200.930004-C251.356 (3)C21-C220.930004-C251.356 (3)C21-H210.9300C1-C21.485 (4)C22-H220.9300C2-C71.409 (4)C24-C291.389 (4)C2-C31.419 (4)C24-C291.389 (4)C3-C41.404 (4)C24-C251.407 (4)C4-C51.373 (4)C25-C261.394 (4)C4-H4A0.9300C26-C271.370 (5)C5-C61.372 (4)C26-H260.9300C5-H5A0.9300C28-C291.362 (5)C6-H60.9300C28-C291.362 (5)C6-H60.9300C28-C291.362 (5)C6-H60.9300C28-H280.9300C8-H80.9300C28-H280.9300C8-H80.9300C28-H280.9300C8-H80.9300C28-H280.9300C8-H80.9300C28-H280.9300C8-H80.9300C28-H280.9300C9-H10169.66 (7)C11-C10-H10120.8N1 ¹ -N1-N3169.09 (8)C12-C11-C10119.1 (3)O2 ¹ -N1-N3100.36 (8)C12-C11-H11
NS-MS ⁱⁱ 1.378 (5)C18-C191.378 (5)NS-H50.8600C18-H180.9300O1-C11.284 (3)C19-C201.352 (5) $02-C3$ 1.339 (3)C19-H190.9300 $02-Ni1^{i1}$ 2.0455 (18)C20-C211.370 (5) $03-C23$ 1.235 (3)C20-H200.9300 $04-C25$ 1.356 (3)C21-H210.9300 $04-C25$ 1.356 (3)C21-H210.9300 $02-C7$ 1.485 (4)C22-H220.9300 $C2-C7$ 1.409 (4)C23-C241.473 (4) $C2-C3$ 1.419 (4)C24-C251.389 (4) $C3-C4$ 1.404 (4)C24-C251.394 (4) $C4-C5$ 1.373 (4)C25-C261.394 (4) $C4-C5$ 1.371 (4)C26-H260.9300 $C5-C6$ 1.372 (4)C26-H260.9300 $C5-H5A$ 0.9300C27-C281.382 (5) $C6-C7$ 1.371 (4)C27-H270.9300 $C5-H5A$ 0.9300C28-C291.362 (5) $C7-H7$ 0.9300C28-H280.9300 $C8-H8$ 0.9300C28-H280.9300 $C8-H8$ 0.9300C28-H280.9300 $N1^{1}-N1-O1$ 79.56 (8)C9-C10-H10120.8 $N1^{1}-N1-N3$ 169.09 (8)C12-C11-H11120.5 $O2^{1}-N1-N3$ 100.36 (8)C12-C11-H11120.5
N5—H50.8600C18—H180.9300O1—C11.284 (3)C19—C201.352 (5)O2—C31.339 (3)C19—H190.9300O2—Ni1 ⁱ 2.0455 (18)C20—C211.370 (5)O3—C231.235 (3)C20—H200.9300O4—C251.356 (3)C21—C221.378 (4)O4—H40.8200C21—H210.9300C2—C71.408 (4)C22—H220.9300C2—C71.409 (4)C24—C291.389 (4)C2—C31.419 (4)C24—C291.389 (4)C3—C41.404 (4)C24—C251.407 (4)C4—H4A0.9300C26—C271.370 (5)C5—C61.372 (4)C26—H260.9300C5—H5A0.9300C27—C281.382 (5)C6—C71.371 (4)C27—H270.9300C5—H5A0.9300C28—C291.362 (5)C7—H70.9300C28—C291.362 (5)C7—H70.9300C28—C291.362 (5)C7—H70.9300C28—C291.362 (5)C7—H70.9300C28—C291.362 (5)C7—H70.9300C28—C291.362 (5)C8—C91.366 (4)C29—H290.9300C8—C91.366 (7)C11—C10—H10120.8O2 ¹ —N1—N3169.09 (8)C12—C11—C10119.1 (3)O2 ¹ —N1—N3169.09 (8)C12—C11—H11120.5O11.19.13100.36 (8)C12—C11—H11120.5
01C11.284 (3)C19C201.352 (5)02C31.339 (3)C19H190.930002Ni11i2.0455 (18)C20C211.370 (5)03C231.235 (3)C20H200.930004C251.356 (3)C21C221.378 (4)04H40.8200C21H210.9300C2C71.485 (4)C22H220.9300C2C71.409 (4)C23C241.473 (4)C2C31.419 (4)C24C291.389 (4)C3C41.404 (4)C24C251.394 (4)C4H4A0.9300C26C271.370 (5)C5C61.372 (4)C26H260.9300C5H5A0.9300C27C281.382 (5)C6-C71.371 (4)C27H270.9300C6-H60.9300C28C291.362 (5)C7-H70.9300C28C291.362 (5)C7-H70.9300C28C291.362 (5)C7-H70.9300C28H280.9300C8C91.366 (4)C29H290.9300C8H80.9300C28H280.9300N1 ¹ -N1I-O179.56 (8)C9C10C11118.3 (3)N1 ¹ -N1I-O3169.09 (8)C12C11C10119.1 (3)O2 ¹ -N1I-N3100.36 (8)C12C11H11120.5O1-N1-N389.96 (8)C10C11H11120.5
$02-C3$ 1.339 (3) $C19-H19$ 0.9300 $02-Ni1^i$ 2.0455 (18) $C20-C21$ 1.370 (5) $03-C23$ 1.235 (3) $C20-H20$ 0.9300 $04-C25$ 1.356 (3) $C21-C22$ 1.378 (4) $04-H4$ 0.8200 $C21-H21$ 0.9300 $C1-C2$ 1.485 (4) $C22-H22$ 0.9300 $C2-C7$ 1.409 (4) $C23-C24$ 1.473 (4) $C2-C3$ 1.419 (4) $C24-C29$ 1.389 (4) $C3-C4$ 1.404 (4) $C24-C25$ 1.407 (4) $C4-C5$ 1.373 (4) $C25-C26$ 1.394 (4) $C4-C5$ 1.372 (4) $C26-H26$ 0.9300 $C5-C6$ 1.372 (4) $C26-H26$ 0.9300 $C5-H5A$ 0.9300 $C27-C28$ 1.382 (5) $C6-C7$ 1.371 (4) $C27-H27$ 0.9300 $C8-C9$ 1.366 (4) $C29-H29$ 0.9300 $C8-C9$ 1.366 (4) $C29-H29$ 0.9300 $C8-C9$ 1.366 (4) $C29-H29$ 0.9300 $C8-H8$ 0.9300 $C2-C10-C11$ 118.3 (3) $N1^i-Ni1-O1$ 79.56 (8) $C9-C10-H10$ 120.8 $O2^i-Ni1-O1$ 169.66 (7) $C11-C10-H10$ 120.8 $O2^i-Ni1-N3$ 100.36 (8) $C12-C11-H11$ 120.5
$O2-Ni1^i$ $2.0455 (18)$ $C20-C21$ $1.370 (5)$ $O3-C23$ $1.235 (3)$ $C20-H20$ 0.9300 $O4-C25$ $1.356 (3)$ $C21-C22$ $1.378 (4)$ $O4-H4$ 0.8200 $C21-H21$ 0.9300 $C1-C2$ $1.485 (4)$ $C22-H22$ 0.9300 $C2-C7$ $1.409 (4)$ $C23-C24$ $1.473 (4)$ $C2-C3$ $1.419 (4)$ $C24-C29$ $1.389 (4)$ $C3-C4$ $1.404 (4)$ $C24-C25$ $1.407 (4)$ $C4-C5$ $1.373 (4)$ $C25-C26$ $1.394 (4)$ $C4-H4A$ 0.9300 $C26-C27$ $1.370 (5)$ $C5-C6$ $1.372 (4)$ $C26-H26$ 0.9300 $C5-H5A$ 0.9300 $C27-C28$ $1.382 (5)$ $C6-C7$ $1.371 (4)$ $C27-H27$ 0.9300 $C5-H6$ 0.9300 $C28-L29$ $1.362 (5)$ $C7-H7$ 0.9300 $C28-H28$ 0.9300 $C8-C9$ $1.366 (4)$ $C29-H29$ 0.9300 $C8-C9$ $1.366 (4)$ $C29-H29$ 0.9300 $C8-H8$ 0.9300 $C1-C10-H10$ 120.8 $O2^i-Ni1-O1$ $169.66 (7)$ $C11-C10-H10$ 120.8 $N1^i-Ni1-N3$ $169.09 (8)$ $C12-C11-H11$ 120.5 $O1-Ni-N3$ $89.96 (8)$ $C10-C11-H11$ 120.5
03C231.235 (3)C20H200.930004C251.356 (3)C21C221.378 (4)04H40.8200C21H210.9300C1C21.485 (4)C22H220.9300C2C71.409 (4)C23C241.473 (4)C2C31.419 (4)C24C291.389 (4)C3C41.404 (4)C24C251.407 (4)C4C51.373 (4)C25C261.394 (4)C4H4A0.9300C26C271.370 (5)C5C61.372 (4)C26H260.9300C5H5A0.9300C27C281.382 (5)C6C71.371 (4)C27H270.9300C6H60.9300C28C291.362 (5)C7H70.9300C28C290.9300C8C91.366 (4)C29H290.9300C8C91.366 (4)C29H290.9300C8H80.9300C1C10C11118.3 (3)N1 ⁱ -Ni1-O179.56 (8)C9C10C11120.8O2 ⁱ -Ni1-O1169.66 (7)C11C10H10120.8O2 ⁱ -Ni1-N3100.36 (8)C12C11H11120.5O1N1-N389.96 (8)C10C11H11120.5
$04-C25$ 1.356 (3) $C21-C22$ 1.378 (4) $04-H4$ 0.8200 $C21-H21$ 0.9300 $C1-C2$ 1.485 (4) $C22-H22$ 0.9300 $C2-C7$ 1.409 (4) $C23-C24$ 1.473 (4) $C2-C3$ 1.419 (4) $C24-C29$ 1.389 (4) $C3-C4$ 1.404 (4) $C24-C25$ 1.407 (4) $C4-C5$ 1.373 (4) $C25-C26$ 1.394 (4) $C4-H4A$ 0.9300 $C26-C27$ 1.370 (5) $C5-C6$ 1.372 (4) $C26-H26$ 0.9300 $C5-H5A$ 0.9300 $C27-C28$ 1.382 (5) $C6-C7$ 1.371 (4) $C27-H27$ 0.9300 $C6-H6$ 0.9300 $C28-C29$ 1.362 (5) $C7-H7$ 0.9300 $C28-H28$ 0.9300 $C8-C9$ 1.366 (4) $C29-H29$ 0.9300 $C8-H8$ 0.9300 $C28-H28$ 0.9300 $N1^i-Ni1-O1$ 79.56 (8) $C9-C10-H10$ 120.8 $N1^i-Ni1-N3$ 169.09 (8) $C12-C11-H11$ 120.5 $O2^i-Ni1-N3$ 100.36 (8) $C12-C11-H11$ 120.5 $O1-Ni1-N3$ 89.96 (8) $C10-C11-H11$ 120.5
O4—H40.8200C21—H210.9300C1—C21.485 (4)C22—H220.9300C2—C71.409 (4)C23—C241.473 (4)C2—C31.419 (4)C24—C291.389 (4)C3—C41.404 (4)C24—C251.407 (4)C4—C51.373 (4)C25—C261.394 (4)C4—H4A0.9300C26—C271.370 (5)C5—C61.372 (4)C26—H260.9300C5—H5A0.9300C27—C281.382 (5)C6—C71.371 (4)C27—H270.9300C6—H60.9300C28—C291.362 (5)C7—H70.9300C28—C291.362 (5)C7—H70.9300C28—H280.9300C8—C91.366 (4)C29—H290.9300C8—H80.9300C11—C11—H11118.3 (3)N1 ⁱ —Ni1—O179.56 (8)C9—C10—H10120.8N1 ⁱ —Ni1—N3169.09 (8)C12—C11—H11120.5O2 ⁱ —Ni1—N3100.36 (8)C12—C11—H11120.5O1—Ni—N389.96 (8)C10—C11—H11120.5
C1-C21.485 (4)C22-H220.9300C2-C71.409 (4)C23-C241.473 (4)C2-C31.419 (4)C24-C291.389 (4)C3-C41.404 (4)C24-C251.407 (4)C4-C51.373 (4)C25-C261.394 (4)C4-H4A0.9300C26-C271.370 (5)C5-C61.372 (4)C26-H260.9300C5-H5A0.9300C27-C281.382 (5)C6-C71.371 (4)C27-H270.9300C6-H60.9300C28-C291.362 (5)C7-H70.9300C28-H280.9300C8-C91.366 (4)C29-H1290.9300C8-H80.9300CN1 ⁱ -Ni1-O1N1 ⁱ -Ni1-O179.56 (8)C9-C10-C11118.3 (3)N1 ⁱ -Ni1-N3169.09 (8)C12-C11-H10120.8N1 ⁱ -Ni1-N3100.36 (8)C12-C11-H11120.5O2 ⁱ -Ni1-N389.96 (8)C10-C11-H11120.5
C2—C7 1.409 (4) C23—C24 1.473 (4) C2—C3 1.419 (4) C24—C29 1.389 (4) C3—C4 1.404 (4) C24—C25 1.407 (4) C4—C5 1.373 (4) C25—C26 1.394 (4) C4—H4A 0.9300 C26—C27 1.370 (5) C5—C6 1.372 (4) C26—H26 0.9300 C5—H5A 0.9300 C27—C28 1.382 (5) C6—C7 1.371 (4) C27—H27 0.9300 C6—H6 0.9300 C28—C29 1.362 (5) C7—H7 0.9300 C28—H28 0.9300 C8—C9 1.366 (4) C29—H29 0.9300 C8—H8 0.9300 C9—C10—C11 118.3 (3) N1 ⁱ —Ni1—O2 ⁱ 90.10 (8) C9—C10—H10 120.8 O2 ⁱ —Ni1—O1 169.66 (7) C11—C10—H10 120.8 N1 ⁱ —Ni1—N3 169.09 (8) C12—C11—C10 119.1 (3) O2 ⁱ —Ni1—N3 100.36 (8) C12—C11—H11 120.5
C2C31.419 (4)C24C291.389 (4)C3C41.404 (4)C24C251.407 (4)C4C51.373 (4)C25C261.394 (4)C4H4A0.9300C26C271.370 (5)C5C61.372 (4)C26H260.9300C5H5A0.9300C27C281.382 (5)C6C71.371 (4)C27H270.9300C6H60.9300C28C291.362 (5)C7H70.9300C28H280.9300C8C91.366 (4)C29H290.9300C8H80.9300C28H280.9300N1 ⁱ Ni1-O179.56 (8)C9C10C11118.3 (3)N1 ⁱ -Ni1-O1169.66 (7)C11C10H10120.8O2 ⁱ Ni1-N3169.09 (8)C12C11C10119.1 (3)O2 ⁱ Ni1-N3100.36 (8)C12C11H11120.5O1Ni1-N389.96 (8)C10C11H11120.5
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C4—C51.373 (4)C25—C261.394 (4)C4—H4A0.9300C26—C271.370 (5)C5—C61.372 (4)C26—H260.9300C5—H5A0.9300C27—C281.382 (5)C6—C71.371 (4)C27—H270.9300C6—H60.9300C28—C291.362 (5)C7—H70.9300C28—H280.9300C8—C91.366 (4)C29—H290.9300C8—H80.9300N1 ⁱ —Ni1—O179.56 (8)C9—C10—C11118.3 (3)N1 ⁱ —Ni1—O1169.66 (7)C11—C10—H10120.8N1 ⁱ —Ni1—N3169.09 (8)C12—C11—C10119.1 (3)O2 ⁱ —Ni1—N3100.36 (8)C12—C11—H11120.5
C4—H4A0.9300C26—C271.370 (5)C5—C61.372 (4)C26—H260.9300C5—H5A0.9300C27—C281.382 (5)C6—C71.371 (4)C27—H270.9300C6—H60.9300C28—C291.362 (5)C7—H70.9300C28—H280.9300C8—C91.366 (4)C29—H290.9300C8—H80.9300C9—C10—C11118.3 (3)N1 ⁱ —Ni1—O2 ⁱ 90.10 (8)C9—C10—C11118.3 (3)N1 ⁱ —Ni1—O179.56 (8)C9—C10—H10120.8O2 ⁱ —Ni1—O1169.66 (7)C11—C10—H10120.8N1 ⁱ —Ni1—N3169.09 (8)C12—C11—C10119.1 (3)O2 ⁱ —Ni1—N3100.36 (8)C12—C11—H11120.5
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C5—H5A0.9300C27—C281.382 (5)C6—C71.371 (4)C27—H270.9300C6—H60.9300C28—C291.362 (5)C7—H70.9300C28—H280.9300C8—C91.366 (4)C29—H290.9300C8—H80.9300C9—C10—C11118.3 (3)N1 ⁱ —Ni1—O2 ⁱ 90.10 (8)C9—C10—H10120.8O2 ⁱ —Ni1—O1169.66 (7)C11—C10—H10120.8N1 ⁱ —Ni1—N3169.09 (8)C12—C11—C10119.1 (3)O2 ⁱ —Ni1—N3100.36 (8)C12—C11—H11120.5O1—Ni1—N389.96 (8)C10—C11—H11120.5
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C8—C91.366 (4)C29—H290.9300C8—H80.93000.93000.9300N1 ⁱ —Ni1—O2 ⁱ 90.10 (8)C9—C10—C11118.3 (3)N1 ⁱ —Ni1—O179.56 (8)C9—C10—H10120.8O2 ⁱ —Ni1—O1169.66 (7)C11—C10—H10120.8N1 ⁱ —Ni1—N3169.09 (8)C12—C11—C10119.1 (3)O2 ⁱ —Ni1—N3100.36 (8)C12—C11—H11120.5O1—Ni1—N389.96 (8)C10—C11—H11120.5
C8—H80.9300N1 ⁱ —Ni1—O2 ⁱ 90.10 (8)C9—C10—C11118.3 (3)N1 ⁱ —Ni1—O179.56 (8)C9—C10—H10120.8O2 ⁱ —Ni1—O1169.66 (7)C11—C10—H10120.8N1 ⁱ —Ni1—N3169.09 (8)C12—C11—C10119.1 (3)O2 ⁱ —Ni1—N3100.36 (8)C12—C11—H11120.5O1—Ni1—N389.96 (8)C10—C11—H11120.5
N1 ⁱ —Ni1—O2 ⁱ 90.10 (8)C9—C10—C11118.3 (3)N1 ⁱ —Ni1—O179.56 (8)C9—C10—H10120.8O2 ⁱ —Ni1—O1169.66 (7)C11—C10—H10120.8N1 ⁱ —Ni1—N3169.09 (8)C12—C11—C10119.1 (3)O2 ⁱ —Ni1—N3100.36 (8)C12—C11—H11120.5O1—Ni1—N389.96 (8)C10—C11—H11120.5
N1 ⁱ —Ni1—O179.56 (8)C9—C10—H10120.8 $O2^{i}$ —Ni1—O1169.66 (7)C11—C10—H10120.8N1 ⁱ —Ni1—N3169.09 (8)C12—C11—C10119.1 (3) $O2^{i}$ —Ni1—N3100.36 (8)C12—C11—H11120.5O1—Ni1—N389.96 (8)C10—C11—H11120.5
$O2^{i}$ —Ni1—O1169.66 (7)C11—C10—H10120.8N1^{i}—Ni1—N3169.09 (8)C12—C11—C10119.1 (3) $O2^{i}$ —Ni1—N3100.36 (8)C12—C11—H11120.5O1—Ni1—N389.96 (8)C10—C11—H11120.5
N1 ⁱ —Ni1—N3 169.09 (8) C12—C11—C10 119.1 (3) O2 ⁱ —Ni1—N3 100.36 (8) C12—C11—H11 120.5 O1—Ni1—N3 89.96 (8) C10—C11—H11 120.5
O2 ⁱ —Ni1—N3 100.36 (8) C12—C11—H11 120.5 O1—Ni1—N3 89.96 (8) C10—C11—H11 120.5
O1—Ni1—N3 89.96 (8) C10—C11—H11 120.5
$N1^{i}$ — $Ni1$ — $N2$ 93.18 (8) $N2$ — $C12$ — $C11$ 123.8 (3)
O2 ⁱ —Ni1—N2 86.83 (8) N2—C12—H12 118.1
O1—Ni1—N2 93.90 (9) C11—C12—H12 118.1
N3—Ni1—N2 90.50 (9) N3—C13—C14 123.0 (3)
N1 ⁱ —Ni1—N4 89.88 (8) N3—C13—H13 118.5
O2 ⁱ —Ni1—N4 89.64 (8) C14—C13—H13 118.5
O1—Ni1—N4 90.12 (9) C15—C14—C13 119.1 (4)
N3—Ni1—N4 87.12 (9) C15—C14—H14 120.5
N2—Ni1—N4 175.33 (8) C13—C14—H14 120.5
21 NH NH 112 0 (0) (14 015 01 (110 9 (0)
$C1 - N1 - N1^{2}$ 113.2 (2) $C14 - C15 - C16$ 118.8 (3)

$\begin{array}{cccccccccccccccccccccccccccccccccccc$	N1 ⁱ —N1—Ni1 ⁱ	113.25 (19)	C16—C15—H15	120.6				
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C12—N2—C8	116.2 (3)	C15—C16—C17	119.0 (3)				
$\begin{array}{llllllllllllllllllllllllllllllllllll$	C12—N2—Ni1	120.89 (18)	С15—С16—Н16	120.5				
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C8—N2—Ni1	122.46 (19)	С17—С16—Н16	120.5				
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C17—N3—C13	117.2 (3)	N3—C17—C16	122.9 (3)				
C13-N3-Nii 117.38 (19) C16-C17-H17 118.6 C18-N4-C22 117.2 (3) N4-C18-C19 122.9 (3) C18-N4-Nii 120.6 (2) N4-C18-H18 118.6 C22-N4-Nii 122.2 (2) C19-C18-H18 118.6 C32-N5-N5 ⁱⁱ 119.0 (3) C20-C19-C18 119.4 (3) C3-N5-H5 120.5 C18-C19-H19 120.3 Ns ⁱⁱ -N5-H5 120.5 C18-C19-H19 120.6 C1-OI-Nii 110.36 (15) C19-C20-C21 118.8 (3) C3-02-Ni1 ⁱ 124.83 (16) C19-C20-H20 120.6 O1-C1-Ni 123.2 (2) C20-C21-H21 120.5 NI-C1-C2 118.8 (2) C20-C21-H21 120.5 NI-C1-C2 118.8 (2) C20-C21-H21 120.5 C7-C2-C1 117.7 (2) N4-C22-C1 122.8 (3) C7-C2-C1 115.1 (2) N3-C23-N5 119.3 (3) O2-C3-C4 118.1 (2) O3-C23-C24 117.5 (3) C3-C2-C1 127.3 (2) C21-C22-H22 118.6 O2-C3-C4 118.1 (2) O3-C23-C24 113.0 (3) C4	C17—N3—Ni1	125.4 (2)	N3—C17—H17	118.6				
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C13—N3—Ni1	117.38 (19)	С16—С17—Н17	118.6				
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C18—N4—C22	117.2 (3)	N4—C18—C19	122.9 (3)				
C22-N4-Ni1 122 2 (2) C19-C18-H18 118.6 C33-N5-N5 th 119.0 (3) C20-C19-C18 119.4 (3) C33-N5-H5 120.5 C20-C19-H19 120.3 Ns ⁱⁿ -N5-H5 120.5 C18-C19-H19 120.3 C1-O1-Ni1 110.36 (15) C19-C20-C21 118.8 (3) C3-02-Ni1 ⁱ 124.83 (16) C19-C20-H20 120.6 O1-C1-N1 123.2 (2) C20-C21-H21 120.5 N1-C1-C2 118.8 (2) C20-C21-H21 120.5 N1-C1-C2 118.0 (2) C22-C21-H21 122.8 (3) C7-C2-C3 117.7 (2) N4-C22-C21 18.6 C3-C2-C1 127.3 (2) C21-C22-H22 18.6 C3-C4 118.1 (2) O3-C23-C24 123.0 (3) C4-C3 122.5 (3) C29-C24-C25 188.2 (3) C5-C4-H4A	C18—N4—Ni1	120.6 (2)	N4—C18—H18	118.6				
C23-NS-NS ⁱⁱ 119.0 (3)C20-C19-C18119.4 (3)C23-NS-H5120.5C20-C19-H19120.3NS ⁱⁱ -NS-H5120.5C18-C19-H19120.3C1-O1-Ni1110.36 (15)C19-C20-C21118.8 (3)C3-O2-Ni1 ⁱ 124.83 (16)C19-C20-H20120.6C25-O4-H4109.5C21-C20-H20120.6O1-C1-N1123.2 (2)C20-C21-C22118.9 (3)O1-C1-C2118.8 (2)C20-C21-H21120.5N1-C1-C2118.0 (2)C22-C21-H21122.8 (3)C7-C2-C3117.7 (2)N4-C22-H22118.6C3-C2-C1127.3 (2)C21-C20-H22118.6C3-C2-C1127.3 (2)C21-C22-H22118.6C3-C2-C2117.5 (2)N5-C23-C24123.0 (3)C4-C3-C2117.5 (3)C29-C24-C23116.8 (3)C3-C4-H4A118.7C29-C24-C23116.8 (3)C3-C4-H4A118.7C29-C24-C23125.0 (3)C5-C4-C4120.5 (3)C4-C25-C26121.1 (3)C6-C5-H5A119.8C26-C25-C24119.5 (3)C4-C5-H5A119.8C26-C25-C24119.7C5-C6-H6120.8C27-C26-H26119.7C5-C6-H6120.8C25-C26-H26119.7C5-C6-H6120.8C25-C26-H26119.7C5-C6-H6120.8C25-C26-H26119.7C5-C6-H6120.8C25-C26-H26119.7C5-C6-H6120.8C26-C27-H27119.8 (4)C7-C6-H6120.8C28-C29-H28120.1	C22—N4—Ni1	122.2 (2)	C19—C18—H18	118.6				
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C23—N5—N5 ⁱⁱ	119.0 (3)	C20—C19—C18	119.4 (3)				
NS ⁱⁱ —NS—H5120.5C18—C19—H19120.3C1—O1—Ni1110.36 (15)C19—C20—C21118.8 (3)C3—O2—Ni1 ⁱ 124.83 (16)C19—C20—H20120.6C25—O4—H4109.5C21—C20—H20120.6O1—C1—N1123.2 (2)C20—C21—H21120.5NI—C1—C2118.8 (2)C20—C21—H21120.5NI—C1—C2118.0 (2)C22—C21112.8 (3)C7—C2—C3117.7 (2)N4—C22—H22118.6C3—C2—C1127.3 (2)C21—C22—H22118.6C3—C2—C1127.3 (2)C21—C22—H22118.6C3—C2—C1127.3 (2)C3—C3—S119.3 (3)O2—C3—C4118.1 (2)O3—C23—N5119.3 (3)O2—C3—C4118.7 C29—C24—C23118.6 (3)C5—C4—H4A118.7C29—C24—C23116.8 (3)C3—C4—H4A118.7C25—C24—C23125.0 (3)C6—C5—C4120.5 (3)O4—C25—C24119.5 (3)C6—C5—H5A119.8C26—C25—C24119.7C5—C6—H6120.8C27—C26—H26119.7C5—C6—H6120.8C25—C24—H27119.9C5—C6—H6120.8C25—C24—H27119.9N2—C8—C9123.7 (3)C28—C27—H27119.9N2—C8—H8118.1C27—C28—H28120.1C9—C8—H8118.9 (3)C28—C29—C24121.8 (4)C10—C9—H9120.6C28—C29—H29119.1C8—C9—H9120.6C28—C29—H29119.1C8—C9—H9120.6C28—C29—H29119.1C8—C9—H912	C23—N5—H5	120.5	С20—С19—Н19	120.3				
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	N5 ⁱⁱ —N5—H5	120.5	C18—C19—H19	120.3				
C3-O2-Ni1i124.83 (16)C19-C20-H20120.6C25-O4-H4109.5C21-C20-H20120.6O1-C1-N1123.2 (2)C20-C21-C22118.9 (3)O1-C1-C2118.8 (2)C20-C21-H21120.5N1-C1-C2118.0 (2)C22-C21-H21120.5C7-C2-C3117.7 (2)N4-C22-C21122.8 (3)C7-C2-C1115.1 (2)N4-C22-H22118.6C3-C2-C1127.3 (2)C21-C22-H22118.6C3-C2-C1127.3 (2)C3-C23-C4113.3 (3)C2-C3-C2124.4 (2)O3-C23-C24123.0 (3)C4-C3-C2117.5 (2)N5-C23-C24117.5 (3)C5-C4-C3122.5 (3)C29-C24-C23116.8 (3)C3-C4-H4A118.7C29-C24-C23116.8 (3)C3-C4-H4A118.7C25-C24-C23116.8 (3)C3-C4-H4A119.8O4-C25-C24119.5 (3)C4-C5-H5A119.8C26-C25-C24119.4 (3)C6-C5-H5A119.8C26-C25-C24119.4 (3)C7-C6-C5118.5 (3)C27-C26-C25120.5 (3)C7-C6-H6120.8C25-C26-H26119.7C5-C6-H6120.8C26-C27-C28120.2 (4)C6-C7-H7118.3C26-C27-C28120.2 (4)C6-C7-H7118.3C26-C27-C28120.2 (4)C6-C7-H7118.3C26-C27-C28120.2 (4)C6-C7-H7118.3C26-C27-C28120.4 (4)C9-C8-H8118.1C27-C28-H28120.1C10-C9-C8118.9 (3)C28-C29-H29119.	C1—O1—Ni1	110.36 (15)	C19—C20—C21	118.8 (3)				
C2504H4109.5C21C20H20120.601C1N1123.2 (2)C20C21C22118.9 (3)01C1C2118.8 (2)C20C21H21120.5N1C1C2118.0 (2)C22C21H21120.5C7C2C3117.7 (2)N4C22C21122.8 (3)C7C2C1115.1 (2)N4C22H22118.6C3C2C1127.3 (2)C21C22H22118.6C3C2124.4 (2)O3C23N5119.3 (3)02C3C2124.4 (2)O3C23C24123.0 (3)C4C3C2117.5 (2)N5C23C24118.2 (3)C5C4H4A118.7C29C24C23116.8 (3)C3C4H4A118.7C25C24C23125.0 (3)C6C5C4120.5 (3)O4C25C24119.5 (3)C4C5H5A119.8O4C25C24119.5 (3)C4C5H5A119.8C26C25C24119.4 (3)C7C6C5118.5 (3)C27C26H26119.7C5C4-H6120.8C25C26-H26119.7C5C5-H6120.8C25C26-H26119.7C5C6-H6120.8C25C26-H26119.7C5C7-H7118.3C26C27H27119.9C2C7-H7118.3C28C27H27119.8 (4)N2C8-H8118.1C29C28-H28120.1C10C9-C8118.9 (3)C28C29H29119.1C8C9-H9120.6C28C29-H29119.1Symmetry codes: (i) -x+1, -y+2, -z; (ii) -x, -y+1, -z+1.L20C29H2	C3—O2—Ni1 ⁱ	124.83 (16)	С19—С20—Н20	120.6				
01C1N1123.2 (2)C20C21C22118.9 (3)01C1C2118.8 (2)C20C21H21120.5N1C1C2118.0 (2)C22C21H21120.5C7C2C3117.7 (2)N4C22C21122.8 (3)C7C2C1115.1 (2)N4C22H22118.6C3C2C1127.3 (2)C21C22H22118.6C3C2C1127.3 (2)C21C22H22118.6C3C2C2124.4 (2)O3C23N5119.3 (3)02C3C2124.4 (2)O3C23C24123.0 (3)C4C3C2117.5 (2)N5C23C24117.5 (3)C5C4C3122.5 (3)C29C24C23116.8 (3)C3C4H4A118.7C25C24125.0 (3)C6C5-C4120.5 (3)O4C25C26121.1 (3)C6C5-H5A119.8O4C25C24119.5 (3)C4C5-H5A119.8C26C25C24119.4 (3)C7C6-L6120.8C25C26119.7C5C6-H6120.8C25C26119.7C5C6-H6120.8C25C26-H26119.7C5C6-H6120.8C25C26-H26119.7C5C6-H6120.8C26C27-H27119.9C2C7-H7118.3C28C27-H27119.8 (4)N2C8-H8118.1C27C28-H28120.1C9C8-H8118.1C27C28-H28120.1C9C8-H8118.1C27C28-H28120.1C9C8-H8118.9C28C29-H29119.1C9C8-H9120.6	С25—О4—Н4	109.5	C21—C20—H20	120.6				
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	01—C1—N1	123.2 (2)	C20—C21—C22	118.9 (3)				
N1C1C2118.0 (2)C22C21H21120.5C7C2C3117.7 (2)N4C22C21122.8 (3)C7C2C1115.1 (2)N4C22H22118.6C3C2C1127.3 (2)C21C22H22118.6O2C3C4118.1 (2)O3C23N5119.3 (3)O2C3C2124.4 (2)O3C23C24123.0 (3)C4C3C2117.5 (2)N5C23C24117.5 (3)C5C4C3122.5 (3)C29C24C23116.8 (3)C3C4H4A118.7C25C24C23125.0 (3)C6C5C4120.5 (3)O4C25C24119.5 (3)C6C5H5A119.8O4C25C24119.5 (3)C7C6-C5118.5 (3)C27C26C25120.5 (3)C7C6H6120.8C27C26H26119.7C5C6H6120.8C25C24-H26119.7C5C6H6120.8C25C26-H26119.7C6C7C2123.4 (3)C26C27C28120.2 (4)C6C7H7118.3C29C28-H28120.1C6C7H7118.3C29C28-H28120.1C9C8H8118.1C29C28-H28120.1C10C9H9120.6C28C29-H29119.1C8C9H9120.6C28C29-H29119.1Symmetry codes: (i) -x+1, -y+2, -z; (ii) -x, -y+1, -z+1.19.919.1	01—C1—C2	118.8 (2)	C20—C21—H21	120.5				
C7-C2-C3117.7 (2)N4-C22-C21122.8 (3)C7-C2-C1115.1 (2)N4-C22-H22118.6C3-C2-C1127.3 (2)C21-C22-H22118.602-C3-C4118.1 (2)03-C23-N5119.3 (3)02-C3-C2124.4 (2)03-C23-C24123.0 (3)C4-C3-C2117.5 (2)N5-C23-C24117.5 (3)C5-C4-C3122.5 (3)C29-C24-C25118.2 (3)C5-C4-H4A118.7C29-C24-C23116.8 (3)C3-C4-H4A118.7C25-C24125.0 (3)C6-C5-C4120.5 (3)O4-C25-C26121.1 (3)C6-C5-H5A119.8O4-C25-C24119.5 (3)C7-C6-C5118.5 (3)C27-C26-C25120.5 (3)C7-C6-C5118.5 (3)C27-C26-C25120.5 (3)C7-C6-H6120.8C25-C26-H26119.7C5-C6-H6120.8C26-C27-C28120.2 (4)C6-C7-C17118.3C26-C27-H27119.9N2-C8-C9123.7 (3)C29-C28-C27119.8 (4)N2-C8-H8118.1C29-C28-H28120.1C9-C8-H8118.1C27-C28-H28120.1C9-C8-H8118.9 (3)C28-C29-H29119.1C10-C9-H9120.6C28-C29-H29119.1Symmetry codes: (i) -x+1, -y+2, -z; (ii) -x, -y+1, -z+1.19.1	N1—C1—C2	118.0 (2)	C22—C21—H21	120.5				
C7C2C1115.1 (2)N4C22H22118.6C3C2C1127.3 (2)C21C22H22118.6O2C3C4118.1 (2)O3C23N5119.3 (3)O2C3C2124.4 (2)O3C23C24123.0 (3)C4C3C2117.5 (2)N5C23C24117.5 (3)C5C4C3122.5 (3)C29C24C25118.2 (3)C5C4H4A118.7C29C24C23116.8 (3)C3C4H4A118.7C25C24C23125.0 (3)C6C5C4120.5 (3)O4C25C26121.1 (3)C6C5H5A119.8O4C25C24119.5 (3)C4C5H5A119.8C26C25C24119.4 (3)C7C6C5118.5 (3)C27C26H26119.7C5C6H6120.8C25C26H26119.7C5C6H6120.8C25C26H26119.7C5C6H6120.8C26C27C28120.2 (4)C6C7C2123.4 (3)C26C27C28120.2 (4)C6C7H7118.3C28C27H27119.9N2C8C9123.7 (3)C29C28H28120.1C9C8H8118.1C29C28H28120.1C9C8H8118.9 (3)C28C29H29119.1C9C8H9120.6C28C29H29119.1Symmetry codes: (i) -x+1, -y+2, -z; (ii) -x, -y+1, -z+1.Symmetry codes: (i) -x+1, -y+2, -z; (ii) -x, -y+1, -z+1.	C7—C2—C3	117.7 (2)	N4—C22—C21	122.8 (3)				
C3-C2-C1127.3 (2)C21-C22-H22118.602-C3-C4118.1 (2)03-C23-N5119.3 (3)02-C3-C2124.4 (2)03-C23-C24123.0 (3)C4-C3-C2117.5 (2)N5-C23-C24117.5 (3)C5-C4-C3122.5 (3)C29-C24-C25118.2 (3)C5-C4-HAA118.7C29-C24-C23116.8 (3)C3-C4-HAA118.7C25-C26121.1 (3)C6-C5-C4120.5 (3)04-C25-C26121.1 (3)C6-C5-H5A119.804-C25-C24119.5 (3)C4-C5-H5A119.8C26-C25-C24119.4 (3)C7-C6-C5118.5 (3)C27-C26-C25120.5 (3)C7-C6-H6120.8C25-C26-H26119.7C5-C6-H6120.8C25-C26-H26119.7C6-C7-C2123.4 (3)C26-C27-C28120.2 (4)C6-C7-H7118.3C26-C27-H27119.9C2-C7-H7118.3C26-C27-H27119.8 (4)N2-C8-C9123.7 (3)C29-C28-H28120.1C9-C8-H8118.1C29-C28-H28120.1C9-C8-H8118.9 (3)C28-C29-H29119.1C9-C8-H9120.6C28-C29-H29119.1C8-C9-H9120.6C28-C29-H29119.1Symmetry codes: (i) -x+1, -y+2, -z; (ii) -x, -y+1, -z+1.UU	C7—C2—C1	115.1 (2)	N4—C22—H22	118.6				
02-C3-C4 $118.1 (2)$ $03-C23-N5$ $119.3 (3)$ $02-C3-C2$ $124.4 (2)$ $03-C23-C24$ $123.0 (3)$ $04-C3-C2$ $117.5 (2)$ $N5-C23-C24$ $117.5 (3)$ $C5-C4-C3$ $122.5 (3)$ $C29-C24-C25$ $118.2 (3)$ $C5-C4-H4A$ 118.7 $C29-C24-C23$ $116.8 (3)$ $C3-C4-H4A$ 118.7 $C25-C24-C23$ $125.0 (3)$ $C6-C5-C4$ $120.5 (3)$ $04-C25-C26$ $121.1 (3)$ $C6-C5-H5A$ 119.8 $04-C25-C24$ $119.5 (3)$ $C4-C5-H5A$ 119.8 $C26-C25-C24$ $119.4 (3)$ $C7-C6-C5$ $118.5 (3)$ $C27-C26-C25$ $120.5 (3)$ $C7-C6-H6$ 120.8 $C25-C26-H26$ 119.7 $C5-C6-H6$ 120.8 $C25-C26-H26$ 119.7 $C5-C6-H6$ 120.8 $C26-C27-C28$ $120.2 (4)$ $C6-C7-H7$ 118.3 $C26-C27-H27$ 119.9 $C2-C7-H7$ 118.3 $C28-C27-H27$ 119.9 $N2-C8-C9$ $123.7 (3)$ $C29-C28-H28$ 120.1 $N2-C8-H8$ 118.1 $C27-C28-H28$ 120.1 $C9-C8-H8$ $118.9 (3)$ $C28-C29-C24$ $121.8 (4)$ $C10-C9-C8$ $118.9 (3)$ $C28-C29-C24$ $121.8 (4)$ $C10-C9-H9$ 120.6 $C28-C29-H29$ 119.1 $Symmetry codes: (i) -x+1, -y+2, -z; (ii) -x, -y+1, -z+1.$ $V=11.9$ $V=11.9$	C3—C2—C1	127.3 (2)	C21—C22—H22	118.6				
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O2—C3—C4	118.1 (2)	O3—C23—N5	119.3 (3)				
C4-C3-C2117.5 (2)N5-C23-C24117.5 (3)C5-C4-C3122.5 (3)C29-C24-C25118.2 (3)C5-C4-H4A118.7C29-C24-C23116.8 (3)C3-C4-H4A118.7C25-C24-C23125.0 (3)C6-C5-C4120.5 (3)O4-C25-C26121.1 (3)C6-C5-H5A119.8O4-C25-C24119.5 (3)C7-C6-C5118.5 (3)C27-C26-C25120.5 (3)C7-C6-H6120.8C27-C26-H26119.7C5-C6-H6120.8C26-C27-C28120.2 (4)C6-C7-H7118.3C26-C27-H27119.9C2-C7-H7118.3C28-C27-H27119.9C2-C7-H7118.1C29-C28-H28120.1C9-C8-H8118.1C27-C28-H28120.1C9-C8-H8118.9 (3)C28-C29-C24121.8 (4)C10-C9-H9120.6C28-C29-H29119.1C8-C9-H9120.6C28-C29-H29119.1C8-C9-H9120.6C28-C29-H29119.1	O2—C3—C2	124.4 (2)	O3—C23—C24	123.0 (3)				
C5C4C3122.5 (3)C29C24C25118.2 (3)C5C4H4A118.7C29C24C23116.8 (3)C3C4H4A118.7C25C24C23125.0 (3)C6C5C4120.5 (3)O4C25C26121.1 (3)C6C5H5A119.8O4C25C24119.5 (3)C4C5H5A119.8C26C25C24119.4 (3)C7C6C5118.5 (3)C27C26C25120.5 (3)C7C6H6120.8C27C26H26119.7C5C6H6120.8C25C24120.2 (4)C6C7C2123.4 (3)C26C27H27119.9C2C7H7118.3C28C27H27119.9C2C7H7118.3C29C28C27119.8 (4)N2C8H8118.1C29C28H28120.1C9C8H8118.9 (3)C28C29C24121.8 (4)C10C9H9120.6C28C29H29119.1C8C9H9120.6C28C29H29119.1C8C9H9120.6C24C29H29119.1	C4—C3—C2	117.5 (2)	N5—C23—C24	117.5 (3)				
C5C4H4A118.7C29C24C23116.8 (3)C3C4H4A118.7C25C24C23125.0 (3)C6C5C4120.5 (3)O4C25C26121.1 (3)C6C5H5A119.8O4C25C24119.5 (3)C4C5H5A119.8C26C25C24119.4 (3)C7C6C5118.5 (3)C27C26C25120.5 (3)C7C6H6120.8C25C26-H26119.7C5C6H6120.8C25C26-H26119.7C6C7C2123.4 (3)C26C27C28120.2 (4)C6C7H7118.3C28C27-H27119.9C2C7H7118.3C29C28-H28120.1C9C8H8118.1C29C28-H28120.1C9C8H8118.9 (3)C28C29C24121.8 (4)C10C9H9120.6C28C29-H29119.1C8C9H9120.6C24C29-H29119.1Symmetry codes: (i) -x+1, -y+2, -z; (ii) -x, -y+1, -z+1.Symmetry codes: (i) -x+1, -y+2, -z; (ii) -x, -y+1, -z+1.	C5—C4—C3	122.5 (3)	C29—C24—C25	118.2 (3)				
C3C4H4A118.7C25C24C23125.0 (3)C6C5C4120.5 (3)04C25C26121.1 (3)C6C5H5A119.804C25C24119.5 (3)C4C5H5A119.8C26C25C24119.4 (3)C7C6C5118.5 (3)C27C26C25120.5 (3)C7C6H6120.8C25C26H26119.7C5C6H6120.8C25C26H26119.7C6C7C2123.4 (3)C26C27C28120.2 (4)C6C7H7118.3C26C27H27119.9C2C7H7118.3C28C27H27119.9N2C8C8118.1C29C28H28120.1C9C8H8118.1C27C28H28120.1C10C9H9120.6C28C29H29119.1C8C9H9120.6C28C29H29119.1C8C9H9120.6C24C29H29119.1Symmetry codes: (i) $-x+1, -y+2, -z;$ (ii) $-x, -y+1, -z+1.$ V	C5—C4—H4A	118.7	C29—C24—C23	116.8 (3)				
C6—C5—C4120.5 (3)04—C25—C26121.1 (3)C6—C5—H5A119.804—C25—C24119.5 (3)C4—C5—H5A119.8C26—C25—C24119.4 (3)C7—C6—C5118.5 (3)C27—C26—C25120.5 (3)C7—C6—H6120.8C27—C26—H26119.7C5—C6—H6120.8C25—C26—H26119.7C6—C7—C2123.4 (3)C26—C27—C28120.2 (4)C6—C7—H7118.3C28—C27—H27119.9C2—C7—H7118.3C29—C28—C27119.8 (4)N2—C8—C9123.7 (3)C29—C28—H28120.1C9—C8—H8118.1C27—C28—H28120.1C10—C9—C8118.9 (3)C28—C29—C24121.8 (4)C10—C9—H9120.6C28—C29—H29119.1C8—C9—H9120.6C24—C29—H29119.1Symmetry codes: (i) -x+1, -y+2, -z; (ii) -x, -y+1, -z+1.Symmetry codes: (i) -x+1, -y+2, -z; (ii) -x, -y+1, -z+1.	C3—C4—H4A	118.7	C25—C24—C23	125.0 (3)				
C6—C5—H5A119.8O4—C25—C24119.5 (3)C4—C5—H5A119.8C26—C25—C24119.4 (3)C7—C6—C5118.5 (3)C27—C26—C25120.5 (3)C7—C6—H6120.8C27—C26—H26119.7C5—C6—H6120.8C25—C26—H26119.7C6—C7—C2123.4 (3)C26—C27—C28120.2 (4)C6—C7—H7118.3C26—C27—H27119.9C2—C7—H7118.3C28—C27—H27119.9N2—C8—C9123.7 (3)C29—C28—C27119.8 (4)N2—C8—H8118.1C29—C28—H28120.1C10—C9—C8118.9 (3)C28—C29—C24121.8 (4)C10—C9—H9120.6C28—C29—H29119.1C8—C9—H9120.6C24—C29—H29119.1Symmetry codes: (i) -x+1, -y+2, -z; (ii) -x, -y+1, -z+1.Symmetry codes: (i) -x+1, -y+2, -z; (ii) -x, -y+1, -z+1.	C6—C5—C4	120.5 (3)	O4—C25—C26	121.1 (3)				
C4—C5—H5A119.8C26—C25—C24119.4 (3)C7—C6—C5118.5 (3)C27—C26—C25120.5 (3)C7—C6—H6120.8C27—C26—H26119.7C5—C6—H6120.8C25—C26—H26119.7C6—C7—C2123.4 (3)C26—C27—C28120.2 (4)C6—C7—H7118.3C26—C27—H27119.9C2—C7—H7118.3C28—C27—H27119.9N2—C8—C9123.7 (3)C29—C28—C27119.8 (4)N2—C8—H8118.1C29—C28—H28120.1C10—C9—C8118.9 (3)C28—C29—C24121.8 (4)C10—C9—H9120.6C28—C29—H29119.1C8—C9—H9120.6C24—C29—H29119.1Symmetry codes: (i) -x+1, -y+2, -z; (ii) -x, -y+1, -z+1.Symmetry codes: (i) -x+1, -y+2, -z; (ii) -x, -y+1, -z+1.	С6—С5—Н5А	119.8	O4—C25—C24	119.5 (3)				
C7—C6—C5118.5 (3)C27—C26—C25120.5 (3)C7—C6—H6120.8C27—C26—H26119.7C5—C6—H6120.8C25—C26—H26119.7C6—C7—C2123.4 (3)C26—C27—C28120.2 (4)C6—C7—H7118.3C26—C27—H27119.9C2—C7—H7118.3C28—C27—H27119.9N2—C8—C9123.7 (3)C29—C28—C27119.8 (4)N2—C8—H8118.1C27—C28—H28120.1C9—C8—H8118.9 (3)C28—C29—C24121.8 (4)C10—C9—C8118.9 (3)C28—C29—H29119.1C8—C9—H9120.6C24—C29—H29119.1Symmetry codes: (i) -x+1, -y+2, -z; (ii) -x, -y+1, -z+1.JJ	C4—C5—H5A	119.8	C26—C25—C24	119.4 (3)				
C7—C6—H6120.8C27—C26—H26119.7C5—C6—H6120.8C25—C26—H26119.7C6—C7—C2123.4 (3)C26—C27—C28120.2 (4)C6—C7—H7118.3C26—C27—H27119.9C2—C7—H7118.3C28—C27—H27119.9N2—C8—C9123.7 (3)C29—C28—C27119.8 (4)N2—C8—H8118.1C29—C28—H28120.1C10—C9—C8118.9 (3)C28—C29—C24121.8 (4)C10—C9—H9120.6C28—C29—H29119.1C8—C9—H9120.6C24—C29—H29119.1Symmetry codes: (i) -x+1, -y+2, -z; (ii) -x, -y+1, -z+1.	C7—C6—C5	118.5 (3)	C27—C26—C25	120.5 (3)				
C5—C6—H6120.8C25—C26—H26119.7C6—C7—C2123.4 (3)C26—C27—C28120.2 (4)C6—C7—H7118.3C26—C27—H27119.9C2—C7—H7118.3C28—C27—H27119.9N2—C8—C9123.7 (3)C29—C28—C27119.8 (4)N2—C8—H8118.1C29—C28—H28120.1C9—C8—H8118.1C27—C28—H28120.1C10—C9—C8118.9 (3)C28—C29—C24121.8 (4)C10—C9—H9120.6C28—C29—H29119.1C8—C9—H9120.6C24—C29—H29119.1Symmetry codes: (i) -x+1, -y+2, -z; (ii) -x, -y+1, -z+1.Symmetry codes: (i) -x+1, -y+2, -z; (ii) -x, -y+1, -z+1.	С7—С6—Н6	120.8	С27—С26—Н26	119.7				
C6—C7—C2123.4 (3)C26—C27—C28120.2 (4)C6—C7—H7118.3C26—C27—H27119.9C2—C7—H7118.3C28—C27—H27119.9N2—C8—C9123.7 (3)C29—C28—C27119.8 (4)N2—C8—H8118.1C29—C28—H28120.1C10—C9—C8118.9 (3)C28—C29—C24121.8 (4)C10—C9—H9120.6C28—C29—H29119.1C8—C9—H9120.6C24—C29—H29119.1Symmetry codes: (i) $-x+1$, $-y+2$, $-z$; (ii) $-x$, $-y+1$, $-z+1$.Image: Constant of the second se	С5—С6—Н6	120.8	С25—С26—Н26	119.7				
C6—C7—H7118.3C26—C27—H27119.9C2—C7—H7118.3C28—C27—H27119.9N2—C8—C9123.7 (3)C29—C28—C27119.8 (4)N2—C8—H8118.1C29—C28—H28120.1C9—C8—H8118.1C27—C28—H28120.1C10—C9—C8118.9 (3)C28—C29—C24121.8 (4)C10—C9—H9120.6C28—C29—H29119.1C8—C9—H9120.6C24—C29—H29119.1Symmetry codes: (i) $-x+1$, $-y+2$, $-z$; (ii) $-x$, $-y+1$, $-z+1$.	C6—C7—C2	123.4 (3)	C26—C27—C28	120.2 (4)				
C2—C7—H7118.3C28—C27—H27119.9N2—C8—C9123.7 (3)C29—C28—C27119.8 (4)N2—C8—H8118.1C29—C28—H28120.1C9—C8—H8118.1C27—C28—H28120.1C10—C9—C8118.9 (3)C28—C29—C24121.8 (4)C10—C9—H9120.6C28—C29—H29119.1C8—C9—H9120.6C24—C29—H29119.1Symmetry codes: (i) $-x+1$, $-y+2$, $-z$; (ii) $-x$, $-y+1$, $-z+1$.V	С6—С7—Н7	118.3	С26—С27—Н27	119.9				
N2—C8—C9123.7 (3)C29—C28—C27119.8 (4)N2—C8—H8118.1C29—C28—H28120.1C9—C8—H8118.1C27—C28—H28120.1C10—C9—C8118.9 (3)C28—C29—C24121.8 (4)C10—C9—H9120.6C28—C29—H29119.1C8—C9—H9120.6C24—C29—H29119.1Symmetry codes: (i) $-x+1$, $-y+2$, $-z$; (ii) $-x$, $-y+1$, $-z+1$.	С2—С7—Н7	118.3	С28—С27—Н27	119.9				
N2—C8—H8 118.1 C29—C28—H28 120.1 C9—C8—H8 118.1 C27—C28—H28 120.1 C10—C9—C8 118.9 (3) C28—C29—C24 121.8 (4) C10—C9—H9 120.6 C28—C29—H29 119.1 C8—C9—H9 120.6 C24—C29—H29 119.1 Symmetry codes: (i) -x+1, -y+2, -z; (ii) -x, -y+1, -z+1. -x+1, -y+2, -z; (ii) -x, -y+1, -z+1. -x+1, -y+2, -z; (ii) -x, -y+1, -z+1.	N2—C8—C9	123.7 (3)	C29—C28—C27	119.8 (4)				
C9—C8—H8 118.1 C27—C28—H28 120.1 C10—C9—C8 118.9 (3) C28—C29—C24 121.8 (4) C10—C9—H9 120.6 C28—C29—H29 119.1 C8—C9—H9 120.6 C24—C29—H29 119.1 Symmetry codes: (i) -x+1, -y+2, -z; (ii) -x, -y+1, -z+1. -x, -y+1, -z+1. -x	N2—C8—H8	118.1	C29—C28—H28	120.1				
C10—C9—C8118.9 (3)C28—C29—C24121.8 (4)C10—C9—H9120.6C28—C29—H29119.1C8—C9—H9120.6C24—C29—H29119.1Symmetry codes: (i) $-x+1$, $-y+2$, $-z$; (ii) $-x$, $-y+1$, $-z+1$.119.1	С9—С8—Н8	118.1	C27—C28—H28	120.1				
C10—C9—H9 120.6 C28—C29—H29 119.1 C8—C9—H9 120.6 C24—C29—H29 119.1 Symmetry codes: (i) -x+1, -y+2, -z; (ii) -x, -y+1, -z+1. 119.1 119.1	С10—С9—С8	118.9 (3)	C28—C29—C24	121.8 (4)				
C8—C9—H9 120.6 C24—C29—H29 119.1 Symmetry codes: (i) $-x+1$, $-y+2$, $-z$; (ii) $-x$, $-y+1$, $-z+1$. 119.1	С10—С9—Н9	120.6	С28—С29—Н29	119.1				
Symmetry codes: (i) $-x+1$, $-y+2$, $-z$; (ii) $-x$, $-y+1$, $-z+1$.	С8—С9—Н9	120.6	С24—С29—Н29	119.1				
	Symmetry codes: (i) $-x+1$, $-y+2$, $-z$; (ii) $-x$, $-y+1$, $-z+1$.							

Hydrogen-bond geometry (Å, °)

D—H···A	<i>D</i> —Н	H···A	$D \cdots A$	D—H···A

O4—H4····O2 ⁱⁱⁱ	0.82	1.72	2.534 (3)	171
Symmetry codes: (iii) $x, y-1, z+1$.				

Fig. 1





