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Crystal structure of bis[2-(1*H*-benzimidazol-2-yl)-4-bromophenolato- $\kappa^2 N^3$,*O*]cobalt(II)

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asymmetric unit of the title Co^{II} complex. The $[Co(C_{13}H_8BrN_2O)_2]$, contains two independent molecules (A and B). In both molecules, the Co^{II} cation is N,O-chelated by two 2-(1H-benzimidazol-2-vl)-4-bromophenolate anions in a distorted tetrahedral geometry. In molecule A, both chelating rings display an envelope conformation, with the flap Co atom lying 0.614 (6) and 0.483 (6) Å from the mean planes of the remaining atoms. In molecule B, both chelating rings are approximately planar, the maximum deviations being 0.039 (4) and 0.076 (3) Å. In the crystal, molecules are linked by classical N-H···O hydrogen bonds and weak C-H···O and $C-H\cdots Br$ hydrogen bonds into a three-dimensional supramolecular network. Extensive $\pi - \pi$ stacking is observed between nearly parallel aromatic rings of adjacent molecules with centroid-centroid distances in the range 3.407 (3)-3.850 (4) Å.

Keywords: crystal structure; cobalt(II); 2-(1*H*-benzimidazol-2-yl)-4bromophenolate anion; hydrogen bonds; π - π stacking.

CCDC reference: 1027432

1. Related literature

For the crystal structures of related metal complexes with the ligand 2-(1*H*-benzoimidazol-2-yl)-4-bromophenolate, see: Li *et al.* (2002); Tong (2007).



V = 4601.9 (5) Å³

Mo $K\alpha$ radiation

 $0.30 \times 0.26 \times 0.20 \text{ mm}$

29475 measured reflections

10549 independent reflections

5904 reflections with $I > 2\sigma(I)$

 $\mu = 4.25 \text{ mm}^-$

T = 293 K

 $R_{\rm int} = 0.053$

Z = 8

2. Experimental

2.1. Crystal data

 $[Co(C_{13}H_8BrN_2O)_2]$ $M_r = 635.16$ Monoclinic, P_{21}/c a = 22.4334 (16) Å b = 8.3598 (6) Å c = 30.0748 (16) Å $\beta = 125.323$ (4)°

2.2. Data collection

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Bruker APEXII CCD
diffractometer
Absorption correction: multi-scan
(SADABS; Bruker, 2001)
T_{min} = 0.258, T_{max} = 0.398
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2.3. Refinement $R[F^2 > 2\sigma(F^2)] = 0.046$ 631 parameters $wR(F^2) = 0.166$ H-atom parameters constrainedS = 0.97 $\Delta \rho_{max} = 0.71 \text{ e Å}^{-3}$ 10549 reflections $\Delta \rho_{min} = -0.65 \text{ e Å}^{-3}$

Table 1Selected bond lengths (Å).

Co1-O2 1.912 (4) Co2-O1	1.930 (4)
Co1-O3 1.903 (4) Co2-O4	1.912 (4)
Co1-N2 1.975 (4) Co2-N6	1.961 (4)
Co1-N3 1.967 (4) Co2-N7	1.957 (4)

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

$D - H \cdot \cdot \cdot A$	D-H	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - H \cdot \cdot \cdot A$
$N1-H1A\cdotsO1^{i}$	0.86	2.19	2.895 (5)	139
N4-H4 A ···O2 ⁱⁱ	0.86	2.09	2.849 (5)	147
N5-H5 A ···O4 ⁱⁱⁱ	0.86	2.41	3.066 (5)	133
N8-H8A···O3 ^{iv}	0.86	2.17	2.808 (5)	131
$C4-H4\cdots Br4^i$	0.93	2.88	3.703 (6)	149
$C6-H6\cdots Br1^{v}$	0.93	2.91	3.685 (6)	142
$C35-H35\cdots O2^{ii}$	0.93	2.54	3.394 (7)	153

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: XU5818).

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Sheldrick, G. M. (2008). Acta Cryst. A64, 112–122.

Tong, Y.-P. (2007). Chin. J. Struct. Chem. 26, 143-145.

supporting information

Acta Cryst. (2014). E70, m363-m364 [doi:10.1107/S1600536814021813]

Crystal structure of bis[2-(1*H*-benzimidazol-2-yl)-4-bromophenolato- $\kappa^2 N^3$,*O*]cobalt(II)

Yan Fan and Zhi-Rong Qu

S1. Comment

The asymmetric unit of the title compound contains two crystallographically independent molecules and bond lengths and angles are in the normal range (Li *et al.*, 2002; Tong, 2007). The Co(II) atom is coordinated by two N atoms and two O atoms to give a distorted tetrahedral geometry (Fig. 1). The benzimidazole and bromophenyl groups are nearly coplanar; the dihedral angle between them is 4.2 (3)°. The angles between the two ligand planes in each independent molecule are 71.66 (5)° and 63.66 (5)°, respectively. The crystal structure is stabilized by N–H···O hydrogen bonds linking molecules into a three-dimensional network structure (Fig. 2). The structure is further stabilized by π - π stacking interactions, the centroid-to-centroid separations are ranged from 3.407 (3) to 3.850 (4) Å.

S2. Experimental

Synthesis of the ligand: The ligands were prepared by the reaction of the addition products of 2-hydroxy-5-bromobenzaldehyde (6 mmol 1.2 g) and NaHSO₃ (6 mmol 0.65 g) were stirred at room temperature in ethanol (25 ml) and a precipitate is formed after 4 h reaction, then, *o*-phenylenediamine (6 mmol, 0.65 g) and 25 ml DMF were added to this mixture. After 2 h reflux the solution was poured into 10-times water. The benzimidazole compound was filtered, dried and crystallized from ethanol.

Synthesis of the complex $[Co(C_{26}H_{16}N_4O_2Br_2)]_2$: 2-(1*H*-benzimidazol-2-yl)-4-bromophenol (0.2 mmol, 58 mg) was dissolved in DMF (6 ml) and CoCl₂.6H₂O (0.1 mmol 24 mg) was dissolved in H₂O (6 ml), and the mixture poured into a 25 ml dicting kettle, then maintaining 393 K for 3 d, allowed to reach room temperate, and red block-shaped crystals suitable for X-ray diffraction were obtained.

S3. Refinement

H atoms were placed in calculated positions with C—H = 0.97-0.93 Å and N—H = 0.86 Å, and refined in riding mode, $U_{iso}(H) = 1.2U_{eq}(C,N)$.



Figure 1

A view of the asymmetric unit of the title compound with atomic numbering scheme. Displacement ellipsoids were drawn at the 30% probability level and all H atoms have been omitted for clarity.



Figure 2

Packing diagram of the title compound viewed along the c axis. Hydrogen bonds are shown as dashed lines.

Bis[2-(1*H*-benzimidazol-2-yl)-4-bromophenolato- $\kappa^2 N^3$, O]cobalt(II)

Crystal data

[Co(C₁₃H₈BrN₂O)₂] $M_r = 635.16$ Monoclinic, $P2_1/c$ a = 22.4334 (16) Å b = 8.3598 (6) Å c = 30.0748 (16) Å $\beta = 125.323$ (4)° V = 4601.9 (5) Å³ Z = 8

Data collection

Bruker APEXII CCD	29475 measured reflections
diffractometer	10549 independent reflections
Radiation source: fine-focus sealed tube	5904 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{\rm int} = 0.053$
φ and ω scans	$\theta_{\rm max} = 27.5^{\circ}, \theta_{\rm min} = 1.1^{\circ}$
Absorption correction: multi-scan	$h = -29 \rightarrow 22$
(SADABS; Bruker, 2001)	$k = -10 \rightarrow 10$
$T_{\min} = 0.258, \ T_{\max} = 0.398$	$l = -36 \rightarrow 39$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier
Least-squares matrix: full	map
$R[F^2 > 2\sigma(F^2)] = 0.046$	Hydrogen site location: inferred from
$wR(F^2) = 0.166$	neighbouring sites
S = 0.97	H-atom parameters constrained
10549 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0908P)^2]$
631 parameters	where $P = (F_o^2 + 2F_c^2)/3$
0 restraints	$(\Delta/\sigma)_{\rm max} = 0.001$
Primary atom site location: structure-invariant	$\Delta \rho_{\rm max} = 0.71 \text{ e } \text{\AA}^{-3}$
direct methods	$\Delta \rho_{\rm min} = -0.65 \text{ e } \text{\AA}^{-3}$

Special details

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

F(000) = 2503

 $\theta = 1.1 - 27.5^{\circ}$

 $\mu = 4.25 \text{ mm}^{-1}$ T = 293 K

Block, red

 $D_{\rm x} = 1.834 {\rm Mg m^{-3}}$

 $0.30 \times 0.26 \times 0.20 \text{ mm}$

Mo *K* α radiation, $\lambda = 0.71073$ Å

Cell parameters from 29475 reflections

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 $(Å^2)$

	x	У	Ζ	$U_{ m iso}$ */ $U_{ m eq}$	
Br1	0.58763 (3)	0.94519 (8)	0.67243 (2)	0.04708 (19)	
Br2	0.96705 (4)	-0.01562 (9)	1.09681 (2)	0.0546 (2)	
Col	0.90832 (4)	0.46833 (10)	0.87113 (3)	0.0345 (2)	
O2	0.85783 (19)	0.6568 (5)	0.86818 (12)	0.0383 (10)	
O3	0.86633 (19)	0.2923 (5)	0.88397 (12)	0.0439 (10)	

		0.5101.(5)		0.0000 (1.0)
N2	0.8868 (2)	0.5101 (5)	0.79854 (15)	0.0278 (10)
N1	0.8152 (2)	0.5734 (5)	0.71102 (15)	0.0298 (10)
H1A	0.7795	0.6141	0.6809	0.036*
N3	1.0079 (2)	0.4220 (5)	0.93502 (15)	0.0321 (10)
N4	1.0909 (2)	0.3509 (5)	1.02030 (15)	0.0312 (10)
H4A	1.1100	0.3093	1.0520	0.037*
C41	0.9158 (3)	0.4410 (7)	0.77260 (19)	0.0354 (13)
C28	1.0753 (3)	0.4820 (7)	0.9510(2)	0.0337 (13)
C36	0.9396 (3)	0.0799 (7)	1.0302 (2)	0.0380 (14)
C40	0.8271 (3)	0.5913 (6)	0.76042 (17)	0.0260 (11)
C27	1.0192 (3)	0.3386 (7)	0.97719 (17)	0.0298 (12)
C46	0.8705 (3)	0.4784 (7)	0.7173 (2)	0.0301 (12)
C45	0.8855 (3)	0 4264 (8)	0.6813(2)	0.0437(15)
H45	0.8550	0.4512	0.6444	0.052*
C48	0.7168(3)	0.7559(7)	0.72527(18)	0.032
H48	0.7050	0.7410	0.72527 (10)	0.0340 (13)
C22	1,1276(2)	0.7419 0.4405 (7)	1.0050(2)	0.041
C33	1.1270(3)	0.4403(7)	1.0030(2)	0.0303(13)
C49	0.0728(3)	0.8449(7)	0.75248(19)	0.0333(13)
C35	0.9864 (3)	0.1691 (7)	1.02/18 (18)	0.0315 (12)
H35	1.0341	0.1807	1.0580	0.038*
C34	0.9655 (3)	0.2465 (7)	0.97832 (17)	0.0303 (12)
C43	0.9927 (3)	0.2955 (8)	0.7576 (2)	0.0488 (16)
H43	1.0336	0.2323	0.7702	0.059*
C44	0.9470 (3)	0.3370 (9)	0.7022 (2)	0.0534 (18)
H44	0.9591	0.3023	0.6790	0.064*
C31	1.2178 (3)	0.5794 (9)	1.0040 (3)	0.0572 (18)
H31	1.2655	0.6161	1.0215	0.069*
C50	0.6885 (3)	0.8666 (7)	0.7841 (2)	0.0408 (14)
H50	0.6569	0.9242	0.7886	0.049*
C47	0.7801 (2)	0.6842 (6)	0.76986 (17)	0.0254 (11)
C42	0.9773 (3)	0.3479 (8)	0.7936 (2)	0.0468 (16)
H42	1.0071	0.3213	0.8304	0.056*
C37	0.8683 (3)	0.0559 (7)	0.9848 (2)	0.0454 (15)
H37	0.8360	-0.0078	0.9869	0.054*
C51	0.7506 (3)	0.8027 (7)	0.82781 (19)	0.0388 (14)
H51	0.7617	0.8204	0.8624	0.047*
C32	1 2000 (3)	0.4847(8)	1.0325(3)	0.0505(17)
H32	1.23/0	0.4526	1.0682	0.0505 (17)
C20	1.2379	0.4520	1.0002	0.001
C53	0.8932(3)	0.2233(7) 0.7121(6)	0.93201(18)	0.0320(13)
C32	0.7979(3)	0.7121(0)	0.02274(10)	0.0292(12)
C29	1.0957 (3)	0.5776 (8)	0.9235 (2)	0.0474 (16)
H29	1.0613	0.6101	0.88//	0.05/*
030	1.1003 (3)	0.6213 (10)	0.9498 (3)	0.063 (2)
H30	1.1808	0.6805	0.9314	0.076*
C38	0.8472 (3)	0.1294 (8)	0.9369 (2)	0.0451 (15)
H38	0.7997	0.1137	0.9063	0.054*
Br3	0.33496 (4)	1.05417 (12)	1.10266 (3)	0.0769 (3)
Br4	0.39831 (4)	0.96643 (12)	0.64170 (3)	0.0711 (3)

010.3195 (2)1.0374 (5)0.89651 (14)0.0451 (11)040.4319 (2)1.0277 (5)0.85430 (14)0.0430 (10)N60.4425 (2)0.8299 (6)0.95111 (15)0.0340 (11)N50.4949 (2)0.7840 (5)1.03884 (15)0.0323 (10)H5A0.50320.78761.07050.039*N70.3160 (2)0.8034 (6)0.81237 (15)0.0339 (11)N80.2534 (2)0.7465 (6)0.72462 (15)0.0356 (11)H8A0.24000.74750.69140.043*C130.3259 (3)1.0325 (7)0.7430 (2)0.0382 (14)C210.3638 (3)0.9497 (7)0.9903 (2)0.0355 (13)C30.5322 (3)0.6743 (7)0.9445 (2)0.0425 (15)H30.51160.69530.90780.01*C190.1575 (3)0.5672 (7)0.7178 (2)0.0435 (15)H190.13120.54320.68090.622*C60.5994 (3)0.6864 (7)1.0561 (2)0.0409 (15)H60.62130.555 (7)1.0370 (2)0.0333 (14)H90.41660.90051.06820.047*C40.552 (3)0.7354 (7)0.9794 (19)0.0314 (12)C50.2528 (3)0.7452 (18)0.0319 (12)C110.4374 (3)0.5597 (7)1.0370 (2)0.0393 (14)H90.41660.90051.06820.047*C150.5282 (3)0.7458 (1)0.0319 (12)C160.5293 (Co2	0.37925 (4)	0.92802 (10)	0.87904 (3)	0.0363 (2)
04 $0.4319 (2)$ $1.0277 (5)$ $0.85430 (14)$ $0.0430 (10)$ N6 $0.4425 (2)$ $0.8299 (6)$ $0.95131 (15)$ $0.0340 (11)$ N5 $0.4949 (2)$ $0.7840 (5)$ $1.0388 (15)$ $0.0323 (10)$ H5A 0.5032 0.7876 1.0705 $0.039*$ N7 $0.3160 (2)$ $0.8034 (6)$ $0.81237 (15)$ $0.0339 (11)$ N8 $0.2534 (2)$ $0.7465 (6)$ $0.72462 (15)$ $0.0336 (11)$ H8A 0.2400 0.7475 0.6014 $0.043*$ C13 $0.3259 (3)$ $1.0325 (7)$ $0.76724 (18)$ $0.0329 (13)$ C14 $0.3128 (3)$ $0.8257 (7)$ $0.76724 (18)$ $0.0325 (13)$ C3 $0.5332 (3)$ $0.6743 (7)$ $0.9903 (2)$ $0.0355 (13)$ C3 $0.5332 (3)$ $0.6743 (7)$ $0.9903 (2)$ $0.0355 (15)$ H3 0.5116 0.6953 0.9078 $0.051*$ C19 $0.1575 (3)$ $0.5672 (7)$ $0.7178 (2)$ $0.445 (15)$ H19 0.1312 0.5432 0.6809 $0.52*$ C6 $0.5994 (3)$ $0.684 (7)$ $1.0551 (2)$ $0.0499 (15)$ H6 0.6213 0.5861 1.0928 $0.049*$ C2 $0.0307 (3)$ $0.9555 (7)$ $1.0370 (2)$ $0.0393 (14)$ C9 $0.3307 (3)$ $0.9585 (7)$ $1.0370 (2)$ $0.0393 (14)$ C14 $0.5948 (3)$ $0.5823 (8)$ $0.9741 (2)$ $0.0478 (16)$ H4 0.6156 0.5406 0.9573 $0.057*$ C15	01	0.3195 (2)	1.0374 (5)	0.89651 (14)	0.0451 (11)
N6 $0.4425 (2)$ $0.8299 (6)$ $0.95131 (15)$ $0.0340 (11)$ N5 $0.4949 (2)$ $0.7840 (5)$ $1.03884 (15)$ $0.0323 (10)$ H5A 0.5032 0.7876 1.0705 $0.039*$ N7 $0.3160 (2)$ $0.8034 (6)$ $0.81237 (15)$ $0.0336 (11)$ N8 $0.2534 (2)$ $0.7465 (6)$ $0.72462 (15)$ $0.0356 (11)$ H8A 0.2400 0.7475 0.6914 $0.043*$ C13 $0.3259 (3)$ $1.0325 (7)$ $0.9430 (2)$ $0.0382 (14)$ C21 $0.3638 (3)$ $0.9139 (7)$ $0.76228 (19)$ $0.0359 (13)$ C14 $0.3128 (3)$ $0.9497 (7)$ $0.9903 (2)$ $0.0325 (13)$ C3 $0.5332 (3)$ $0.6743 (7)$ $0.9445 (2)$ $0.0425 (15)$ H3 0.5116 0.6953 0.9078 $0.051*$ C19 $0.1575 (3)$ $0.5672 (7)$ $0.7178 (2)$ $0.0435 (15)$ H9 0.1312 0.5432 0.6809 $0.052*$ C6 $0.5994 (3)$ $0.6084 (7)$ $1.0561 (2)$ $0.049*$ C2 $0.5037 (3)$ $0.7554 (7)$ $0.97079 (18)$ $0.0314 (12)$ C9 $0.3807 (3)$ $0.9555 (7)$ $1.0370 (2)$ $0.0393 (14)$ H9 0.4166 0.9005 1.0682 $0.047*$ C4 $0.5948 (3)$ $0.5823 (8)$ $0.9741 (2)$ $0.478 (16)$ H4 0.6155 0.5406 0.9573 $0.57*$ C15 $0.2582 (3)$ $0.7447 (7)$ $0.8984 (19)$ $0.0334 (13)$ C26 0.421	O4	0.4319 (2)	1.0277 (5)	0.85430 (14)	0.0430 (10)
NS 0.4949 (2) 0.7840 (5) 1.03884 (15) 0.0323 (10) H5A 0.502 0.7876 1.0705 0.039* N7 0.3160 (2) 0.8034 (6) 0.81237 (15) 0.0339 (11) N8 0.2534 (2) 0.7465 (6) 0.72462 (15) 0.0326 (11) H8A 0.2400 0.7475 0.6914 0.0432* C13 0.3259 (3) 1.0325 (7) 0.76286 (19) 0.0352 (13) C21 0.3638 (3) 0.9497 (7) 0.9903 (2) 0.0355 (13) C3 0.5332 (3) 0.6743 (7) 0.7445 (2) 0.0425 (15) H3 0.5116 0.6953 0.9078 0.051* C19 0.1575 (3) 0.5672 (7) 1.7178 (2) 0.0435 (15) H19 0.1312 0.5432 0.6809 0.052* C6 0.5994 (3) 0.5823 (8) 0.9797 (8) 0.0314 (12) C9 0.3807 (3) 0.555 (7) 1.0370 (2) 0.0393 (14) C9 0.3807 (3) 0.5523 (8) 0.9741 (2) <t< td=""><td>N6</td><td>0.4425 (2)</td><td>0.8299 (6)</td><td>0.95131 (15)</td><td>0.0340 (11)</td></t<>	N6	0.4425 (2)	0.8299 (6)	0.95131 (15)	0.0340 (11)
H5A0.50320.78761.07050.039*N70.3160 (2)0.8034 (6)0.81237 (15)0.0336 (11)N80.2534 (2)0.7465 (6)0.72462 (15)0.0356 (11)H8A0.24000.74750.69140.043*C130.3259 (3)1.0325 (7)0.9430 (2)0.0359 (13)C140.3128 (3)0.9257 (7)0.76286 (19)0.0359 (13)C140.3128 (3)0.9257 (7)0.76724 (18)0.0324 (13)C80.3808 (3)0.9497 (7)0.9903 (2)0.0355 (15)C80.3308 (3)0.6743 (7)0.9445 (2)0.0425 (15)H30.51160.69530.90780.051*C190.1575 (3)0.5672 (7)0.7178 (2)0.0435 (15)H190.13120.54320.68090.052*C60.5994 (3)0.6884 (7)1.09280.049*C20.5037 (3)0.7354 (7)0.97079 (18)0.0314 (12)C90.3807 (3)0.9555 (7)1.0370 (2)0.0393 (14)H90.41660.90051.06820.047*C40.5948 (3)0.5823 (8)0.9741 (2)0.04478 (16)H40.61560.54060.95730.057*C150.2582 (3)0.7042 (7)0.79894 (19)0.0344 (13)C260.4212 (3)1.0058 (8)1.0377 (2)0.0445 (16)C170.1765 (3)0.5397 (7)0.8052 (3)0.047*C260.2284 (3)1.0748 (9)0.7502 (3)0.057*	N5	0.4949 (2)	0.7840 (5)	1.03884 (15)	0.0323 (10)
N7 0.3160 (2) 0.8034 (6) 0.81237 (15) 0.0339 (11) $N8$ 0.2534 (2) 0.7465 (6) 0.72462 (15) 0.0356 (1) $H8A$ 0.2400 0.7475 0.6914 $0.043*$ $C13$ 0.3259 (3) 1.0325 (7) 0.9430 (2) 0.0382 (14) $C21$ 0.3638 (3) 0.9139 (7) 0.76286 (19) 0.0359 (13) $C14$ 0.3128 (3) 0.8257 (7) 0.76724 (18) 0.0324 (13) $C8$ 0.3808 (3) 0.9497 (7) 0.9903 (2) 0.0355 (13) $C3$ 0.5332 (3) 0.6743 (7) 0.9445 (2) 0.0425 (15) $H3$ 0.5116 0.6953 0.9078 $0.051*$ $C19$ 0.1575 (3) 0.5672 (7) 0.7178 (2) 0.0435 (15) $H19$ 0.1312 0.5432 0.6809 $0.052*$ $C6$ 0.5994 (3) 0.6084 (7) 1.0561 (2) $0.049*$ (15) $H6$ 0.6213 0.5861 1.0928 $0.049*$ $C2$ 0.5037 (3) 0.7354 (7) 0.97079 (18) 0.0314 (12) $C9$ 0.3807 (3) 0.9555 (7) 1.0370 (2) 0.0393 (14) $H9$ 0.4166 0.9005 1.0682 $0.047*$ $C4$ 0.5948 (3) 0.5823 (8) 0.9774 (2) 0.0478 (16) $H4$ 0.6156 0.5406 0.9573 $0.057*$ $C15$ 0.2382 (3) 0.7042 (7) 0.79894 (19) 0.3341 (13) $C26$ 0.4212 (3) 1.0588 (8) 0.8068 (2) $0.$	H5A	0.5032	0.7876	1.0705	0.039*
N8 0.2534 (2) 0.7465 (6) 0.72462 (15) 0.0356 (11) H8A 0.2400 0.7475 0.6914 0.043* C13 0.3259 (3) 1.0325 (7) 0.9430 (2) 0.0382 (14) C21 0.3638 (3) 0.9139 (7) 0.76226 (19) 0.0359 (13) C14 0.3128 (3) 0.8257 (7) 0.76724 (18) 0.0325 (13) C8 0.3808 (3) 0.9497 (7) 0.9903 (2) 0.0425 (15) H3 0.5116 0.6953 0.9078 0.0425 (15) H3 0.5116 0.6684 (7) 1.0561 (2) 0.0435 (15) H19 0.1312 0.5432 0.6809 0.052* C6 0.5994 (3) 0.6584 (7) 1.0561 (2) 0.0499 (15) H6 0.6213 0.5855 (7) 1.0370 (2) 0.0339 (14) C9 0.3807 (3) 0.555 (7) 1.0370 (2) 0.0339 (14) C9 0.3807 (3) 0.555 (7) 0.6822 0.047* C4 0.5948 (3) 0.5824 (2) 0.0474 (12)	N7	0.3160 (2)	0.8034 (6)	0.81237 (15)	0.0339 (11)
H8A 0.2400 0.7475 0.6914 0.043^* C13 $0.3259(3)$ $1.0325(7)$ $0.9430(2)$ $0.0382(14)$ C21 $0.3638(3)$ $0.9139(7)$ $0.76286(19)$ $0.0359(13)$ C14 $0.3128(3)$ $0.8257(7)$ $0.76224(18)$ $0.0324(13)$ C8 $0.3808(3)$ $0.9497(7)$ $0.9903(2)$ $0.0355(13)$ C3 $0.5332(3)$ $0.6743(7)$ $0.9445(2)$ $0.0425(15)$ H3 0.5116 0.6953 0.9078 0.051^* C19 $0.1575(3)$ $0.5672(7)$ $0.7178(2)$ $0.0435(15)$ H19 0.1312 0.5432 0.6809 0.052^* C6 $0.5994(3)$ $0.6084(7)$ $1.0561(2)$ $0.049(15)$ H6 0.6213 0.5861 1.0928 0.049^* C2 $0.5037(3)$ $0.7354(7)$ $0.97079(18)$ $0.0314(12)$ C9 $0.3807(3)$ $0.9555(7)$ $1.0370(2)$ $0.393(14)$ H9 0.4166 0.9005 1.0682 0.047^* C4 $0.5948(3)$ $0.5823(8)$ $0.9741(2)$ $0.0478(16)$ H4 0.6156 0.5406 0.9573 0.057^* C15 $0.2582(3)$ $0.7042(7)$ $0.79894(19)$ $0.0344(13)$ C26 $0.4212(3)$ $1.0058(8)$ $0.8068(2)$ $0.0404(15)$ C1 $0.4374(3)$ $0.8591(7)$ $0.8052(3)$ $0.0471(16)$ H7 0.1611 0.9947 0.8253 0.057^* C26 $0.2582(3)$ $1.0748(9)$ $0.7502(3)$ 0.0475	N8	0.2534 (2)	0.7465 (6)	0.72462 (15)	0.0356 (11)
C13 $0.3259 (3)$ $1.0325 (7)$ $0.9430 (2)$ $0.0382 (14)$ C21 $0.03638 (3)$ $0.9139 (7)$ $0.76286 (19)$ $0.0359 (13)$ C14 $0.3128 (3)$ $0.8257 (7)$ $0.76724 (18)$ $0.0324 (13)$ C8 $0.3808 (3)$ $0.9497 (7)$ $0.9903 (2)$ $0.0355 (13)$ C3 $0.5332 (3)$ $0.6743 (7)$ $0.9445 (2)$ $0.0425 (15)$ H3 0.5116 0.6953 0.9078 $0.051*$ C19 $0.1575 (3)$ $0.5672 (7)$ $0.7178 (2)$ $0.0435 (15)$ H19 0.1312 0.5432 0.6809 $0.052*$ C6 $0.5994 (3)$ $0.6084 (7)$ $1.0561 (2)$ $0.0409 (15)$ H6 0.6213 $0.7354 (7)$ $0.97079 (18)$ $0.0314 (12)$ C9 $0.3807 (3)$ $0.9555 (7)$ $1.0370 (2)$ $0.0393 (14)$ H9 0.4166 0.9005 1.0682 $0.047*$ C4 $0.5948 (3)$ $0.5823 (8)$ $0.9741 (2)$ $0.0478 (16)$ H4 0.6156 0.5406 0.9573 $0.057*$ C15 $0.2582 (3)$ $0.7042 (7)$ $0.79894 (19)$ $0.0344 (13)$ C26 $0.4212 (3)$ $1.0058 (8)$ $0.8068 (2)$ $0.0404 (15)$ C17 $0.1765 (3)$ $0.5397 (7)$ $0.8052 (3)$ $0.057*$ C16 $0.3293 (3)$ $1.0395 (8)$ $1.0377 (2)$ $0.0445 (16)$ C17 $0.1765 (3)$ $0.5397 (7)$ $0.8052 (3)$ $0.057*$ C26 $0.4212 (3)$ $1.0748 (9)$ $0.7532 (3)$ $0.057*$	H8A	0.2400	0.7475	0.6914	0.043*
C21 0.3638 (3) 0.9139 (7) 0.76286 (19) 0.0359 (13)C14 0.3128 (3) 0.8257 (7) 0.76724 (18) 0.0324 (13)C8 0.3808 (3) 0.9497 (7) 0.9903 (2) 0.0355 (13)C3 0.5332 (3) 0.6743 (7) 0.9445 (2) 0.0425 (15)H3 0.5116 0.6953 0.9078 0.051^* C19 0.1575 (3) 0.5672 (7) 0.7178 (2) 0.0435 (15)H19 0.1312 0.5432 0.6809 0.52^* C6 0.5994 (3) 0.6084 (7) 1.0561 (2) 0.0409 (15)H6 0.6213 0.5861 1.0928 0.049^* C2 0.5037 (3) 0.7354 (7) 0.97079 (18) 0.0314 (12)C9 0.3807 (3) 0.9555 (7) 1.0370 (2) 0.0437 (16)H4 0.6156 0.5406 0.9573 0.057^* C4 0.5948 (3) 0.5823 (8) 0.9741 (2) 0.0478 (16)H4 0.6156 0.5406 0.9573 0.057^* C15 0.2582 (3) 0.7042 (7) 0.99257 (18) 0.0319 (12)C10 0.3293 (3) 1.0395 (8) 1.0377 (2) 0.0455 (16)C17 0.1765 (3) 0.5397 (7) 0.8052 (3) 0.057^* C20 0.2184 (3) 1.0395 (8) 1.0377 (2) 0.0455 (16)C17 0.1523 0.0574 0.5506 (8) 1.0284 (2) 0.0303 (12)C24 0.4628 (3) 1.0748 (9) 0.7502 (3) 0.0521 (17)<	C13	0.3259 (3)	1.0325 (7)	0.9430 (2)	0.0382 (14)
C14 $0.3128 (3)$ $0.8257 (7)$ $0.76724 (18)$ $0.0324 (13)$ C8 $0.3808 (3)$ $0.9497 (7)$ $0.9903 (2)$ $0.0355 (13)$ C3 $0.5332 (3)$ $0.6743 (7)$ $0.9445 (2)$ $0.0425 (15)$ H3 0.5116 0.6953 0.9078 $0.051*$ C19 $0.1575 (3)$ $0.5672 (7)$ $0.7178 (2)$ $0.0435 (15)$ H19 0.1312 0.5432 0.6809 $0.052*$ C6 $0.5994 (3)$ $0.6084 (7)$ $1.0561 (2)$ $0.0409 (15)$ H6 0.6213 0.5861 1.0928 $0.049*$ C2 $0.5037 (3)$ $0.7354 (7)$ $0.97079 (18)$ $0.0314 (12)$ C9 $0.3807 (3)$ $0.9555 (7)$ $1.0370 (2)$ $0.0393 (14)$ H9 0.4166 0.9005 1.0682 $0.047*$ C4 $0.5948 (3)$ $0.5823 (8)$ $0.9741 (2)$ $0.0478 (16)$ H4 0.6156 0.5406 0.9573 $0.057*$ C15 $0.2582 (3)$ $0.7042 (7)$ $0.79894 (19)$ $0.0344 (13)$ C26 $0.4212 (3)$ $1.0058 (8)$ $0.8068 (2)$ $0.0404 (15)$ C1 $0.4327 (3)$ $0.3591 (7)$ $0.99257 (18)$ $0.0319 (12)$ C10 $0.3293 (3)$ $1.0395 (8)$ $1.0377 (2)$ $0.0455 (16)$ C17 $0.1765 (3)$ $0.5397 (7)$ $0.8052 (3)$ $0.0471 (16)$ H17 0.1611 0.4947 0.8253 $0.057*$ C20 $0.2184 (3)$ $0.5484 (6)$ $0.7434 (2)$ $0.0303 (12)$ C24 0	C21	0.3638 (3)	0.9139 (7)	0.76286 (19)	0.0359 (13)
C8 $0.3808 (3)$ $0.9497 (7)$ $0.9903 (2)$ $0.0355 (13)$ C3 $0.5332 (3)$ $0.6743 (7)$ $0.9445 (2)$ $0.0425 (15)$ H3 0.5116 0.6953 0.9078 $0.051*$ C19 $0.1575 (3)$ $0.5672 (7)$ $0.7178 (2)$ $0.0435 (15)$ H19 0.1312 0.5432 0.6809 $0.052*$ C6 $0.5994 (3)$ $0.6084 (7)$ $1.0561 (2)$ $0.0409 (15)$ H6 0.6213 0.5861 1.0928 $0.049*$ C2 $0.5037 (3)$ $0.7354 (7)$ $0.97079 (18)$ $0.0314 (12)$ C9 $0.3807 (3)$ $0.9555 (7)$ $1.0370 (2)$ $0.0393 (14)$ H9 0.4166 0.9005 1.0682 $0.047*$ C4 $0.5948 (3)$ $0.5823 (8)$ $0.9741 (2)$ $0.0478 (16)$ H4 0.6156 0.5406 0.9573 $0.057*$ C15 $0.2582 (3)$ $0.7042 (7)$ $0.99257 (18)$ $0.0319 (12)$ C10 $0.3293 (3)$ $1.0395 (8)$ $1.0377 (2)$ $0.0455 (16)$ C17 $0.1765 (3)$ $0.5397 (7)$ $0.8052 (3)$ $0.0471 (16)$ H17 0.1611 0.4947 0.8253 $0.057*$ C20 $0.2184 (3)$ $0.6648 (6)$ $0.7434 (2)$ $0.0303 (12)$ C24 $0.4628 (3)$ $1.0748 (9)$ $0.7502 (3)$ $0.0571 (17)$ H24 0.4951 1.1293 0.7457 $0.062*$ C5 $0.6266 (3)$ $0.5506 (8)$ $1.0284 (2)$ $0.0478 (16)$ H5 0.6684 0.6871	C14	0.3128 (3)	0.8257 (7)	0.76724 (18)	0.0324 (13)
C3 0.5332 (3) 0.6743 (7) 0.9445 (2) 0.0425 (15)H3 0.5116 0.6953 0.9078 $0.051*$ C19 0.1575 (3) 0.5672 (7) 0.7178 (2) 0.0435 (15)H19 0.1312 0.5432 0.6809 $0.052*$ C6 0.5994 (3) 0.6084 (7) 1.0561 (2) 0.0409 (15)H6 0.6213 0.5861 1.0928 $0.049*$ C2 0.5037 (3) 0.7354 (7) 0.97079 (18) 0.0314 (12)C9 0.3807 (3) 0.9555 (7) 1.0370 (2) 0.0393 (14)H9 0.4166 0.9005 1.0682 $0.047*$ C4 0.5948 (3) 0.5823 (8) 0.9741 (2) 0.0478 (16)H4 0.6156 0.5406 0.9573 $0.057*$ C15 0.2582 (3) 0.7042 (7) 0.79894 (19) 0.0344 (13)C26 0.4212 (3) 1.0058 (8) 0.8068 (2) 0.0404 (15)C1 0.4374 (3) 0.8591 (7) 0.99257 (18) 0.0319 (12)C10 0.3293 (3) 1.0395 (8) 1.0377 (2) 0.0455 (16)C17 0.1765 (3) 0.5397 (7) 0.8052 (3) $0.057*$ C20 0.2184 (3) 0.6648 (6) 0.7434 (2) 0.0478 (16)H17 0.1611 0.4947 0.8253 $0.057*$ C20 0.2184 (3) 0.5506 (8) 1.0284 (2) 0.0457 (16)C24 0.4628 (3) 0.5506 (8) 1.0284 (2) 0.0454 (16)H25 0.6664	C8	0.3808 (3)	0.9497 (7)	0.9903 (2)	0.0355 (13)
H30.51160.69530.90780.051*C190.1575 (3)0.5672 (7)0.7178 (2)0.0435 (15)H190.13120.54320.68090.052*C60.5994 (3)0.6084 (7)1.0561 (2)0.0409 (15)H60.62130.58611.09280.049*C20.5037 (3)0.7354 (7)0.97079 (18)0.0314 (12)C90.3807 (3)0.9555 (7)1.0370 (2)0.0393 (14)H90.41660.90051.06820.047*C40.5948 (3)0.5823 (8)0.9741 (2)0.0478 (16)H40.61560.54060.95730.057*C150.2582 (3)0.7042 (7)0.79894 (19)0.0344 (13)C260.4212 (3)1.0058 (8)0.8068 (2)0.0404 (15)C10.4374 (3)0.8591 (7)0.99257 (18)0.0319 (12)C100.3293 (3)1.0395 (8)1.0377 (2)0.0455 (16)C170.1765 (3)0.5397 (7)0.8052 (3)0.0471 (16)H170.16110.49470.82530.057*C200.2184 (3)0.6648 (6)0.7434 (2)0.0303 (12)C240.4628 (3)1.0748 (9)0.7502 (3)0.0521 (17)H240.49511.12930.74570.062*C50.6266 (3)0.5506 (8)1.0284 (2)0.0478 (16)H50.66840.48731.04710.057*C70.5373 (3)0.7018 (7)0.8302 (2)0.0381 (13)H160.2	C3	0.5332 (3)	0.6743 (7)	0.9445 (2)	0.0425 (15)
C190.1575 (3)0.5672 (7)0.7178 (2)0.0435 (15)H190.13120.54320.68090.052*C60.5994 (3)0.6084 (7)1.0561 (2)0.0409 (15)H60.62130.58611.09280.049*C20.5037 (3)0.7354 (7)0.97079 (18)0.0314 (12)C90.3807 (3)0.9555 (7)1.0370 (2)0.0393 (14)H90.41660.90051.06820.047*C40.5948 (3)0.5823 (8)0.9741 (2)0.0478 (16)H40.61560.54060.95730.057*C150.2582 (3)0.7042 (7)0.79894 (19)0.0344 (13)C260.4212 (3)1.0058 (8)0.8068 (2)0.0404 (15)C10.4374 (3)0.8591 (7)0.99257 (18)0.0319 (12)C100.3293 (3)1.0395 (8)1.0377 (2)0.0455 (16)C170.1765 (3)0.5397 (7)0.8052 (3)0.0471 (16)H170.16110.49470.82530.057*C200.2184 (3)0.6648 (6)0.7434 (2)0.0303 (12)C240.4628 (3)1.0748 (9)0.7502 (3)0.0521 (17)H240.49511.12930.74570.062*C50.6266 (3)0.5506 (8)1.0284 (2)0.0478 (16)H50.66840.6371 (7)0.8302 (2)0.0331 (13)H60.26280.65820.86730.046*C20.3593 (3)0.9059 (9)0.7142 (2)0.0454 (16)H2	H3	0.5116	0.6953	0.9078	0.051*
H19 0.1312 0.5432 0.6809 $0.052*$ C6 0.5994 (3) 0.6084 (7) 1.0561 (2) 0.0409 (15)H6 0.6213 0.5861 1.0928 $0.049*$ C2 0.5037 (3) 0.7354 (7) 0.97079 (18) 0.0314 (12)C9 0.3807 (3) 0.9555 (7) 1.0370 (2) 0.0393 (14)H9 0.4166 0.9005 1.0682 $0.047*$ C4 0.5948 (3) 0.5823 (8) 0.9741 (2) 0.0478 (16)H4 0.6156 0.5406 0.9573 $0.057*$ C15 0.2582 (3) 0.7042 (7) 0.79894 (19) 0.0344 (13)C26 0.4212 (3) 1.0058 (8) 0.8068 (2) 0.0404 (15)C1 0.4374 (3) 0.8591 (7) 0.99257 (18) 0.0319 (12)C10 0.3293 (3) 1.0395 (8) 1.0377 (2) 0.0455 (16)C17 0.1765 (3) 0.5397 (7) 0.8052 (3) 0.0471 (16)H17 0.1611 0.4947 0.8253 $0.057*$ C20 0.2184 (3) 1.0748 (9) 0.7502 (3) 0.0521 (17)H24 0.4951 1.1293 0.7457 $0.062*$ C5 0.6266 (3) 0.5506 (8) 1.0284 (2) 0.0478 (16)H5 0.6684 0.4873 1.0471 $0.057*$ C7 0.5373 (3) 0.718 (7) 0.8302 (2) 0.0381 (13)H5 0.6684 0.6851 $0.024*$ 0.6582 0.6673 C4 0.2228 0.6582	C19	0.1575 (3)	0.5672 (7)	0.7178 (2)	0.0435 (15)
C6 $0.5994 (3)$ $0.6084 (7)$ $1.0561 (2)$ $0.0409 (15)$ H6 0.6213 0.5861 1.0928 $0.049*$ C2 $0.5037 (3)$ $0.7354 (7)$ $0.97079 (18)$ $0.0314 (12)$ C9 $0.3807 (3)$ $0.9555 (7)$ $1.0370 (2)$ $0.0393 (14)$ H9 0.4166 0.9005 1.0682 $0.047*$ C4 $0.5948 (3)$ $0.5823 (8)$ $0.9741 (2)$ $0.0478 (16)$ H4 0.6156 0.5406 0.9573 $0.057*$ C15 $0.2582 (3)$ $0.7042 (7)$ $0.79894 (19)$ $0.0344 (13)$ C26 $0.4212 (3)$ $1.0058 (8)$ $0.8068 (2)$ $0.0404 (15)$ C1 $0.4374 (3)$ $0.8591 (7)$ $0.99257 (18)$ $0.0319 (12)$ C10 $0.3293 (3)$ $1.0395 (8)$ $1.0377 (2)$ $0.0455 (16)$ C17 $0.1765 (3)$ $0.5397 (7)$ $0.8052 (3)$ $0.0471 (16)$ H17 0.1611 0.4947 0.8253 $0.057*$ C20 $0.2184 (3)$ $0.6648 (6)$ $0.7434 (2)$ $0.0303 (12)$ C24 $0.4628 (3)$ $1.0748 (9)$ $0.7502 (3)$ $0.0521 (17)$ H24 0.4951 1.1293 0.7457 $0.662*$ C5 $0.6266 (3)$ $0.5506 (8)$ $1.0284 (2)$ $0.0478 (16)$ H5 0.6684 0.4873 1.0471 $0.057*$ C7 $0.5373 (3)$ $0.7018 (7)$ $1.02606 (18)$ $0.0307 (12)$ C25 $0.4695 (3)$ $1.0851 (8)$ $0.7981 (2)$ $0.0445 (16)$ H25 0	H19	0.1312	0.5432	0.6809	0.052*
H6 0.6213 0.5861 1.0928 0.049^* C2 $0.5037 (3)$ $0.7354 (7)$ $0.97079 (18)$ $0.0314 (12)$ C9 $0.3807 (3)$ $0.9555 (7)$ $1.0370 (2)$ $0.0393 (14)$ H9 0.4166 0.9005 1.0682 0.047^* C4 $0.5948 (3)$ $0.5823 (8)$ $0.9741 (2)$ $0.0478 (16)$ H4 0.6156 0.5406 0.9573 0.057^* C15 $0.2582 (3)$ $0.7042 (7)$ $0.79894 (19)$ $0.0344 (13)$ C26 $0.4212 (3)$ $1.0058 (8)$ $0.8068 (2)$ $0.4044 (15)$ C1 $0.4374 (3)$ $0.8591 (7)$ $0.99257 (18)$ $0.0319 (12)$ C10 $0.3293 (3)$ $1.0395 (8)$ $1.0377 (2)$ $0.0455 (16)$ C17 $0.1765 (3)$ $0.5397 (7)$ $0.8052 (3)$ $0.0471 (16)$ H17 0.1611 0.4947 0.8253 0.057^* C20 $0.2184 (3)$ $0.6648 (6)$ $0.7434 (2)$ $0.0303 (12)$ C24 $0.4628 (3)$ $1.0748 (9)$ $0.7502 (3)$ $0.0521 (17)$ H24 0.4951 1.1293 0.7457 0.062^* C5 $0.6266 (3)$ $0.5506 (8)$ $1.0284 (2)$ $0.0478 (16)$ H5 0.6684 0.4873 1.0471 0.057^* C7 $0.5373 (3)$ $0.7018 (7)$ $1.02606 (18)$ $0.0307 (12)$ C25 $0.4695 (3)$ $1.0851 (8)$ $0.7981 (2)$ 0.0464^* C16 $0.2367 (3)$ 0.6582 0.8673 0.066^* C12 $0.2744 (3$	C6	0.5994 (3)	0.6084 (7)	1.0561 (2)	0.0409 (15)
C2 $0.5037 (3)$ $0.7354 (7)$ $0.97079 (18)$ $0.0314 (12)$ $C9$ $0.3807 (3)$ $0.9555 (7)$ $1.0370 (2)$ $0.0393 (14)$ $H9$ 0.4166 0.9005 1.0682 $0.047*$ $C4$ $0.5948 (3)$ $0.5823 (8)$ $0.9741 (2)$ $0.0478 (16)$ $H4$ 0.6156 0.5406 0.9573 $0.057*$ $C15$ $0.2582 (3)$ $0.7042 (7)$ $0.79894 (19)$ $0.0344 (13)$ $C26$ $0.4212 (3)$ $1.0058 (8)$ $0.8068 (2)$ $0.4040 (15)$ $C1$ $0.4374 (3)$ $0.8591 (7)$ $0.99257 (18)$ $0.0319 (12)$ $C10$ $0.3293 (3)$ $1.0395 (8)$ $1.0377 (2)$ $0.0455 (16)$ $C17$ $0.1765 (3)$ $0.5397 (7)$ $0.8052 (3)$ $0.4471 (16)$ $H17$ 0.1611 0.4947 0.8253 $0.057*$ $C20$ $0.2184 (3)$ $0.6648 (6)$ $0.7434 (2)$ $0.0303 (12)$ $C24$ $0.4628 (3)$ $1.0748 (9)$ $0.7502 (3)$ $0.0521 (17)$ $H24$ 0.4951 1.1293 0.7457 $0.062*$ $C5$ $0.6266 (3)$ $0.5506 (8)$ $1.0284 (2)$ $0.0478 (16)$ $H5$ 0.6684 0.4873 1.0471 $0.057*$ $C7$ $0.5373 (3)$ $0.7018 (7)$ $1.02606 (18)$ $0.0307 (12)$ $C25$ $0.4695 (3)$ $1.0851 (8)$ $0.7981 (2)$ 0.0464 $H2$ $0.4695 (3)$ $1.0851 (8)$ $0.7981 (2)$ 0.0464 $H2$ 0.2374 $1.1173 (8)$ $0.9458 (2)$ 0	H6	0.6213	0.5861	1.0928	0.049*
C9 $0.3807 (3)$ $0.9555 (7)$ $1.0370 (2)$ $0.0393 (14)$ H9 0.4166 0.9005 1.0682 $0.047*$ C4 $0.5948 (3)$ $0.5823 (8)$ $0.9741 (2)$ $0.0478 (16)$ H4 0.6156 0.5406 0.9573 $0.057*$ C15 $0.2582 (3)$ $0.7042 (7)$ $0.79894 (19)$ $0.0344 (13)$ C26 $0.4212 (3)$ $1.0058 (8)$ $0.8068 (2)$ $0.0404 (15)$ C1 $0.4374 (3)$ $0.8591 (7)$ $0.99257 (18)$ $0.0319 (12)$ C10 $0.3293 (3)$ $1.0395 (8)$ $1.0377 (2)$ $0.0455 (16)$ C17 $0.1765 (3)$ $0.5397 (7)$ $0.8052 (3)$ $0.0471 (16)$ H17 0.1611 0.4947 0.8253 $0.057*$ C20 $0.2184 (3)$ $0.6648 (6)$ $0.7434 (2)$ $0.0303 (12)$ C24 $0.4628 (3)$ $1.0748 (9)$ $0.7502 (3)$ $0.0521 (17)$ H24 0.4951 1.1293 0.7457 $0.062*$ C5 $0.6266 (3)$ $0.5506 (8)$ $1.0284 (2)$ $0.0478 (16)$ H5 0.6684 0.4873 1.0471 $0.057*$ C7 $0.5373 (3)$ $0.7018 (7)$ $1.02606 (18)$ $0.0307 (12)$ C25 $0.4695 (3)$ $1.0851 (8)$ $0.7981 (2)$ $0.0454 (16)$ H25 0.5072 1.1465 0.8673 $0.046*$ C16 $0.2367 (3)$ $0.959 (9)$ $0.7142 (2)$ $0.0464 (16)$ H22 0.3219 0.8463 0.6853 $0.056*$ C12 $0.2744 (3)$ <t< td=""><td>C2</td><td>0.5037 (3)</td><td>0.7354 (7)</td><td>0.97079 (18)</td><td>0.0314 (12)</td></t<>	C2	0.5037 (3)	0.7354 (7)	0.97079 (18)	0.0314 (12)
H90.41660.90051.06820.047*C40.5948 (3)0.5823 (8)0.9741 (2)0.0478 (16)H40.61560.54060.95730.057*C150.2582 (3)0.7042 (7)0.79894 (19)0.0344 (13)C260.4212 (3)1.0058 (8)0.8068 (2)0.0404 (15)C10.4374 (3)0.8591 (7)0.99257 (18)0.0319 (12)C100.3293 (3)1.0395 (8)1.0377 (2)0.0455 (16)C170.1765 (3)0.5397 (7)0.8052 (3)0.0471 (16)H170.16110.49470.82530.057*C200.2184 (3)0.6648 (6)0.7434 (2)0.0303 (12)C240.4628 (3)1.0748 (9)0.7502 (3)0.0521 (17)H240.49511.12930.74570.062*C50.6266 (3)0.5506 (8)1.0284 (2)0.04478 (16)H50.66840.48731.04710.057*C70.5373 (3)0.7018 (7)1.02606 (18)0.0307 (12)C250.4695 (3)1.0851 (8)0.7981 (2)0.0454 (16)H250.50721.14650.86730.046*C160.2367 (3)0.65820.86730.046*C220.3593 (3)0.9059 (9)0.7142 (2)0.0464 (16)H220.2744 (3)1.1173 (8)0.9458 (2)0.0457 (16)H220.23741.1239 (8)0.9918 (2)0.0457 (16)C130.4072 (3)0.9819 (8)0.7081 (2)0.0457 (16)<	C9	0.3807 (3)	0.9555 (7)	1.0370 (2)	0.0393 (14)
C4 0.5948 (3) 0.5823 (8) 0.9741 (2) 0.0478 (16)H4 0.6156 0.5406 0.9573 $0.057*$ C15 0.2582 (3) 0.7042 (7) 0.79894 (19) 0.0344 (13)C26 0.4212 (3) 1.0058 (8) 0.8068 (2) 0.0404 (15)C1 0.4374 (3) 0.8591 (7) 0.99257 (18) 0.0319 (12)C10 0.3293 (3) 1.0395 (8) 1.0377 (2) 0.0455 (16)C17 0.1765 (3) 0.5397 (7) 0.8052 (3) 0.0471 (16)H17 0.1611 0.4947 0.8253 $0.057*$ C20 0.2184 (3) 1.0748 (9) 0.7502 (3) 0.0521 (17)H24 0.4628 (3) 1.0748 (9) 0.7502 (3) 0.0521 (17)H24 0.4951 1.1293 0.7457 $0.062*$ C5 0.6266 (3) 0.5506 (8) 1.0284 (2) 0.0478 (16)H5 0.6684 0.4873 1.0471 $0.057*$ C7 0.5373 (3) 0.7018 (7) 1.02606 (18) 0.0307 (12)C25 0.4695 (3) 1.0851 (8) 0.7981 (2) 0.0454 (16)H25 0.5072 1.1465 0.8261 $0.054*$ C16 0.2367 (3) 0.6582 0.8673 $0.046*$ C22 0.3593 (3) 0.9059 (9) 0.7142 (2) 0.0445 (16)H26 0.2374 1.1715 0.9150 $0.051*$ C16 0.2374 1.1715 0.9150 $0.051*$ C22 0.3293 (3) 0.9819	H9	0.4166	0.9005	1.0682	0.047*
H40.61560.54060.95730.057*C150.2582 (3)0.7042 (7)0.79894 (19)0.0344 (13)C260.4212 (3)1.0058 (8)0.8068 (2)0.0404 (15)C10.4374 (3)0.8591 (7)0.99257 (18)0.0319 (12)C100.3293 (3)1.0395 (8)1.0377 (2)0.0455 (16)C170.1765 (3)0.5397 (7)0.8052 (3)0.0471 (16)H170.16110.49470.82530.057*C200.2184 (3)0.6648 (6)0.7434 (2)0.0303 (12)C240.4628 (3)1.0748 (9)0.7502 (3)0.0521 (17)H240.49511.12930.74570.062*C50.6266 (3)0.5506 (8)1.0284 (2)0.0478 (16)H50.66840.48731.04710.057*C70.5373 (3)0.7018 (7)1.02606 (18)0.0307 (12)C250.4695 (3)1.0851 (8)0.7981 (2)0.0454 (16)H250.50721.14650.82610.054*C160.2367 (3)0.6371 (7)0.8302 (2)0.0381 (13)H60.26280.65820.86730.046*C220.3593 (3)0.9059 (9)0.7142 (2)0.0464 (16)H220.32190.84630.68530.056*C120.2744 (3)1.1173 (8)0.9458 (2)0.0425 (14)H120.23741.1239 (8)0.9918 (2)0.0445 (15)H110.24161.18440.99250.053*C180.	C4	0.5948 (3)	0.5823 (8)	0.9741 (2)	0.0478 (16)
C15 $0.2582 (3)$ $0.7042 (7)$ $0.79894 (19)$ $0.0344 (13)$ C26 $0.4212 (3)$ $1.0058 (8)$ $0.8068 (2)$ $0.0404 (15)$ C1 $0.4374 (3)$ $0.8591 (7)$ $0.99257 (18)$ $0.0319 (12)$ C10 $0.3293 (3)$ $1.0395 (8)$ $1.0377 (2)$ $0.0455 (16)$ C17 $0.1765 (3)$ $0.5397 (7)$ $0.8052 (3)$ $0.0471 (16)$ H17 0.1611 0.4947 0.8253 $0.057*$ C20 $0.2184 (3)$ $0.6648 (6)$ $0.7434 (2)$ $0.0303 (12)$ C24 $0.4628 (3)$ $1.0748 (9)$ $0.7502 (3)$ $0.0521 (17)$ H24 0.4951 1.1293 0.7457 $0.062*$ C5 $0.6266 (3)$ $0.5506 (8)$ $1.0284 (2)$ $0.0478 (16)$ H5 0.6684 0.4873 1.0471 $0.057*$ C7 $0.5373 (3)$ $0.7018 (7)$ $1.02606 (18)$ $0.3007 (12)$ C25 $0.4695 (3)$ $1.0851 (8)$ $0.7981 (2)$ $0.0454 (16)$ H25 0.5072 1.1465 0.8261 $0.054*$ C16 $0.2367 (3)$ $0.9059 (9)$ $0.7142 (2)$ $0.0464 (16)$ H22 0.3219 0.8463 0.6853 $0.056*$ C12 $0.2744 (3)$ $1.1173 (8)$ $0.9458 (2)$ $0.0457 (16)$ C11 $0.2759 (3)$ $1.1239 (8)$ $0.9918 (2)$ $0.0445 (15)$ H11 0.2416 1.1844 0.9925 $0.053*$	H4	0.6156	0.5406	0.9573	0.057*
C26 $0.4212 (3)$ $1.0058 (8)$ $0.8068 (2)$ $0.0404 (15)$ C1 $0.4374 (3)$ $0.8591 (7)$ $0.99257 (18)$ $0.0319 (12)$ C10 $0.3293 (3)$ $1.0395 (8)$ $1.0377 (2)$ $0.0455 (16)$ C17 $0.1765 (3)$ $0.5397 (7)$ $0.8052 (3)$ $0.0471 (16)$ H17 0.1611 0.4947 0.8253 $0.057*$ C20 $0.2184 (3)$ $0.6648 (6)$ $0.7434 (2)$ $0.0303 (12)$ C24 $0.4628 (3)$ $1.0748 (9)$ $0.7502 (3)$ $0.0521 (17)$ H24 0.4951 1.1293 0.7457 $0.062*$ C5 $0.6266 (3)$ $0.5506 (8)$ $1.0284 (2)$ $0.0478 (16)$ H5 0.6684 0.4873 1.0471 $0.057*$ C7 $0.5373 (3)$ $0.7018 (7)$ $1.02606 (18)$ $0.0307 (12)$ C25 $0.4695 (3)$ $1.0851 (8)$ $0.7981 (2)$ $0.0454 (16)$ H25 0.5072 1.1465 0.8261 $0.054*$ C16 $0.2367 (3)$ 0.6582 0.8673 $0.046*$ C22 $0.3593 (3)$ $0.9059 (9)$ $0.7142 (2)$ $0.0464 (16)$ H22 0.3219 0.8463 0.6853 $0.056*$ C12 $0.2744 (3)$ $1.173 (8)$ $0.9458 (2)$ $0.0457 (16)$ C11 $0.2759 (3)$ $1.1239 (8)$ $0.9918 (2)$ $0.0445 (15)$ H11 0.2416 1.1844 0.9925 $0.053*$	C15	0.2582 (3)	0.7042 (7)	0.79894 (19)	0.0344 (13)
C1 $0.4374 (3)$ $0.8591 (7)$ $0.99257 (18)$ $0.0319 (12)$ C10 $0.3293 (3)$ $1.0395 (8)$ $1.0377 (2)$ $0.0455 (16)$ C17 $0.1765 (3)$ $0.5397 (7)$ $0.8052 (3)$ $0.0471 (16)$ H17 0.1611 0.4947 0.8253 $0.057*$ C20 $0.2184 (3)$ $0.6648 (6)$ $0.7434 (2)$ $0.0303 (12)$ C24 $0.4628 (3)$ $1.0748 (9)$ $0.7502 (3)$ $0.0521 (17)$ H24 0.4951 1.1293 0.7457 $0.062*$ C5 $0.6266 (3)$ $0.5506 (8)$ $1.0284 (2)$ $0.0478 (16)$ H5 0.6684 0.4873 1.0471 $0.057*$ C7 $0.5373 (3)$ $0.7018 (7)$ $1.02606 (18)$ $0.0307 (12)$ C25 $0.4695 (3)$ $1.0851 (8)$ $0.7981 (2)$ $0.0454 (16)$ H25 0.5072 1.1465 0.8261 $0.054*$ C16 $0.2367 (3)$ 0.6582 0.8673 $0.046*$ C22 $0.3593 (3)$ $0.9059 (9)$ $0.7142 (2)$ $0.0464 (16)$ H22 $0.2744 (3)$ $1.173 (8)$ $0.9458 (2)$ $0.0425 (14)$ H12 0.2374 1.1715 0.9150 $0.051*$ C23 $0.4072 (3)$ $0.9819 (8)$ $0.7081 (2)$ $0.0445 (15)$ H11 0.2416 1.1844 0.9925 $0.053*$ C18 $0.1387 (3)$ $0.5089 (8)$ $0.7500 (3)$ $0.0480 (16)$	C26	0.4212 (3)	1.0058 (8)	0.8068 (2)	0.0404 (15)
C100.3293 (3)1.0395 (8)1.0377 (2)0.0455 (16)C170.1765 (3)0.5397 (7)0.8052 (3)0.0471 (16)H170.16110.49470.82530.057*C200.2184 (3)0.6648 (6)0.7434 (2)0.0303 (12)C240.4628 (3)1.0748 (9)0.7502 (3)0.0521 (17)H240.49511.12930.74570.062*C50.6266 (3)0.5506 (8)1.0284 (2)0.0478 (16)H50.66840.48731.04710.057*C70.5373 (3)0.7018 (7)1.02606 (18)0.307 (12)C250.4695 (3)1.0851 (8)0.7981 (2)0.04454 (16)H250.50721.14650.82610.054*C160.2367 (3)0.6371 (7)0.8302 (2)0.0381 (13)H160.26280.65820.86730.046*C220.3593 (3)0.9059 (9)0.7142 (2)0.0464 (16)H220.32190.84630.68530.056*C120.2744 (3)1.1173 (8)0.9458 (2)0.0425 (14)H120.23741.17150.91500.051*C230.4072 (3)0.9819 (8)0.7081 (2)0.0457 (16)C110.2759 (3)1.1239 (8)0.9918 (2)0.0445 (15)H110.24161.18440.99250.053*C180.1387 (3)0.5089 (8)0.7500 (3)0.0480 (16)	C1	0.4374 (3)	0.8591 (7)	0.99257 (18)	0.0319 (12)
C170.1765 (3)0.5397 (7)0.8052 (3)0.0471 (16)H170.16110.49470.82530.057*C200.2184 (3)0.6648 (6)0.7434 (2)0.0303 (12)C240.4628 (3)1.0748 (9)0.7502 (3)0.0521 (17)H240.49511.12930.74570.062*C50.6266 (3)0.5506 (8)1.0284 (2)0.0478 (16)H50.66840.48731.04710.057*C70.5373 (3)0.7018 (7)1.02606 (18)0.0307 (12)C250.4695 (3)1.0851 (8)0.7981 (2)0.0454 (16)H250.50721.14650.82610.054*C160.2367 (3)0.6371 (7)0.8302 (2)0.0381 (13)H160.26280.65820.86730.046*C220.3593 (3)0.9059 (9)0.7142 (2)0.0464 (16)H220.2744 (3)1.1173 (8)0.9458 (2)0.0425 (14)H120.23741.17150.91500.051*C230.4072 (3)0.9819 (8)0.7081 (2)0.0445 (15)H110.24161.18440.99250.053*C180.1387 (3)0.5089 (8)0.7500 (3)0.0480 (16)	C10	0.3293 (3)	1.0395 (8)	1.0377 (2)	0.0455 (16)
H170.16110.49470.82530.057*C200.2184 (3)0.6648 (6)0.7434 (2)0.0303 (12)C240.4628 (3)1.0748 (9)0.7502 (3)0.0521 (17)H240.49511.12930.74570.062*C50.6266 (3)0.5506 (8)1.0284 (2)0.0478 (16)H50.66840.48731.04710.057*C70.5373 (3)0.7018 (7)1.02606 (18)0.0307 (12)C250.4695 (3)1.0851 (8)0.7981 (2)0.0454 (16)H250.50721.14650.82610.054*C160.2367 (3)0.6371 (7)0.8302 (2)0.0381 (13)H160.26280.65820.86730.046*C220.3593 (3)0.9059 (9)0.7142 (2)0.0464 (16)H220.2744 (3)1.1173 (8)0.9458 (2)0.0425 (14)H120.23741.17150.91500.051*C230.4072 (3)0.9819 (8)0.7081 (2)0.0445 (15)H110.24161.18440.99250.053*C180.1387 (3)0.5089 (8)0.7500 (3)0.0480 (16)	C17	0.1765 (3)	0.5397 (7)	0.8052 (3)	0.0471 (16)
C20 $0.2184 (3)$ $0.6648 (6)$ $0.7434 (2)$ $0.0303 (12)$ C24 $0.4628 (3)$ $1.0748 (9)$ $0.7502 (3)$ $0.0521 (17)$ H24 0.4951 1.1293 0.7457 $0.062*$ C5 $0.6266 (3)$ $0.5506 (8)$ $1.0284 (2)$ $0.0478 (16)$ H5 0.6684 0.4873 1.0471 $0.057*$ C7 $0.5373 (3)$ $0.7018 (7)$ $1.02606 (18)$ $0.0307 (12)$ C25 $0.4695 (3)$ $1.0851 (8)$ $0.7981 (2)$ $0.0454 (16)$ H25 0.5072 1.1465 0.8261 $0.054*$ C16 $0.2367 (3)$ $0.6371 (7)$ $0.8302 (2)$ $0.0381 (13)$ H16 0.2628 0.6582 0.8673 $0.046*$ C22 $0.3593 (3)$ $0.9059 (9)$ $0.7142 (2)$ $0.0454 (16)$ H22 $0.2744 (3)$ $1.1173 (8)$ $0.9458 (2)$ $0.0425 (14)$ H12 0.2374 1.1715 0.9150 $0.051*$ C23 $0.4072 (3)$ $0.9819 (8)$ $0.7081 (2)$ $0.0445 (15)$ H11 0.2416 1.1844 0.9925 $0.053*$ C18 $0.1387 (3)$ $0.5089 (8)$ $0.7500 (3)$ $0.0480 (16)$	H17	0.1611	0.4947	0.8253	0.057*
C240.4628 (3)1.0748 (9)0.7502 (3)0.0521 (17)H240.49511.12930.74570.062*C50.6266 (3)0.5506 (8)1.0284 (2)0.0478 (16)H50.66840.48731.04710.057*C70.5373 (3)0.7018 (7)1.02606 (18)0.0307 (12)C250.4695 (3)1.0851 (8)0.7981 (2)0.0454 (16)H250.50721.14650.82610.054*C160.2367 (3)0.6371 (7)0.8302 (2)0.0381 (13)H160.26280.65820.86730.046*C220.3593 (3)0.9059 (9)0.7142 (2)0.0464 (16)H220.32190.84630.68530.056*C120.2744 (3)1.1173 (8)0.9458 (2)0.0425 (14)H120.23741.17150.91500.051*C230.4072 (3)0.9819 (8)0.7081 (2)0.0445 (15)H110.24161.18440.99250.053*C180.1387 (3)0.5089 (8)0.7500 (3)0.0480 (16)	C20	0.2184 (3)	0.6648 (6)	0.7434 (2)	0.0303 (12)
H240.49511.12930.74570.062*C50.6266 (3)0.5506 (8)1.0284 (2)0.0478 (16)H50.66840.48731.04710.057*C70.5373 (3)0.7018 (7)1.02606 (18)0.0307 (12)C250.4695 (3)1.0851 (8)0.7981 (2)0.0454 (16)H250.50721.14650.82610.054*C160.2367 (3)0.6371 (7)0.8302 (2)0.0381 (13)H160.26280.65820.86730.046*C220.3593 (3)0.9059 (9)0.7142 (2)0.0464 (16)H220.32190.84630.68530.056*C120.2744 (3)1.1173 (8)0.9458 (2)0.0425 (14)H120.23741.17150.91500.051*C230.4072 (3)0.9819 (8)0.7081 (2)0.0445 (15)H110.24161.18440.99250.053*C180.1387 (3)0.5089 (8)0.7500 (3)0.0480 (16)	C24	0.4628 (3)	1.0748 (9)	0.7502 (3)	0.0521 (17)
C50.6266 (3)0.5506 (8)1.0284 (2)0.0478 (16)H50.66840.48731.04710.057*C70.5373 (3)0.7018 (7)1.02606 (18)0.0307 (12)C250.4695 (3)1.0851 (8)0.7981 (2)0.0454 (16)H250.50721.14650.82610.054*C160.2367 (3)0.6371 (7)0.8302 (2)0.0381 (13)H160.26280.65820.86730.046*C220.3593 (3)0.9059 (9)0.7142 (2)0.0464 (16)H220.32190.84630.68530.056*C120.2744 (3)1.1173 (8)0.9458 (2)0.0425 (14)H120.23741.17150.91500.051*C230.4072 (3)0.9819 (8)0.7081 (2)0.0445 (15)H110.24161.18440.99250.053*C180.1387 (3)0.5089 (8)0.7500 (3)0.0480 (16)	H24	0.4951	1.1293	0.7457	0.062*
H50.66840.48731.04710.057*C70.5373 (3)0.7018 (7)1.02606 (18)0.0307 (12)C250.4695 (3)1.0851 (8)0.7981 (2)0.0454 (16)H250.50721.14650.82610.054*C160.2367 (3)0.6371 (7)0.8302 (2)0.0381 (13)H160.26280.65820.86730.046*C220.3593 (3)0.9059 (9)0.7142 (2)0.0464 (16)H220.32190.84630.68530.056*C120.2744 (3)1.1173 (8)0.9458 (2)0.0425 (14)H120.23741.17150.91500.051*C230.4072 (3)0.9819 (8)0.7081 (2)0.0445 (15)H110.24161.18440.99250.053*C180.1387 (3)0.5089 (8)0.7500 (3)0.0480 (16)	C5	0.6266 (3)	0.5506 (8)	1.0284 (2)	0.0478 (16)
C70.5373 (3)0.7018 (7)1.02606 (18)0.0307 (12)C250.4695 (3)1.0851 (8)0.7981 (2)0.0454 (16)H250.50721.14650.82610.054*C160.2367 (3)0.6371 (7)0.8302 (2)0.0381 (13)H160.26280.65820.86730.046*C220.3593 (3)0.9059 (9)0.7142 (2)0.0464 (16)H220.32190.84630.68530.056*C120.2744 (3)1.1173 (8)0.9458 (2)0.0425 (14)H120.23741.17150.91500.051*C230.4072 (3)0.9819 (8)0.7081 (2)0.0445 (15)H110.24161.18440.99250.053*C180.1387 (3)0.5089 (8)0.7500 (3)0.0480 (16)	Н5	0.6684	0.4873	1.0471	0.057*
C250.4695 (3)1.0851 (8)0.7981 (2)0.0454 (16)H250.50721.14650.82610.054*C160.2367 (3)0.6371 (7)0.8302 (2)0.0381 (13)H160.26280.65820.86730.046*C220.3593 (3)0.9059 (9)0.7142 (2)0.0464 (16)H220.32190.84630.68530.056*C120.2744 (3)1.1173 (8)0.9458 (2)0.0425 (14)H120.23741.17150.91500.051*C230.4072 (3)0.9819 (8)0.7081 (2)0.0445 (15)H110.24161.18440.99250.053*C180.1387 (3)0.5089 (8)0.7500 (3)0.0480 (16)	C7	0.5373 (3)	0.7018 (7)	1.02606 (18)	0.0307 (12)
H250.50721.14650.82610.054*C160.2367 (3)0.6371 (7)0.8302 (2)0.0381 (13)H160.26280.65820.86730.046*C220.3593 (3)0.9059 (9)0.7142 (2)0.0464 (16)H220.32190.84630.68530.056*C120.2744 (3)1.1173 (8)0.9458 (2)0.0425 (14)H120.23741.17150.91500.051*C230.4072 (3)0.9819 (8)0.7081 (2)0.0445 (15)H110.24161.18440.99250.053*C180.1387 (3)0.5089 (8)0.7500 (3)0.0480 (16)	C25	0.4695 (3)	1.0851 (8)	0.7981 (2)	0.0454 (16)
C160.2367 (3)0.6371 (7)0.8302 (2)0.0381 (13)H160.26280.65820.86730.046*C220.3593 (3)0.9059 (9)0.7142 (2)0.0464 (16)H220.32190.84630.68530.056*C120.2744 (3)1.1173 (8)0.9458 (2)0.0425 (14)H120.23741.17150.91500.051*C230.4072 (3)0.9819 (8)0.7081 (2)0.0457 (16)C110.2759 (3)1.1239 (8)0.9918 (2)0.0445 (15)H110.24161.18440.99250.053*C180.1387 (3)0.5089 (8)0.7500 (3)0.0480 (16)	H25	0.5072	1.1465	0.8261	0.054*
H160.26280.65820.86730.046*C220.3593 (3)0.9059 (9)0.7142 (2)0.0464 (16)H220.32190.84630.68530.056*C120.2744 (3)1.1173 (8)0.9458 (2)0.0425 (14)H120.23741.17150.91500.051*C230.4072 (3)0.9819 (8)0.7081 (2)0.0457 (16)C110.2759 (3)1.1239 (8)0.9918 (2)0.0445 (15)H110.24161.18440.99250.053*C180.1387 (3)0.5089 (8)0.7500 (3)0.0480 (16)	C16	0.2367 (3)	0.6371 (7)	0.8302 (2)	0.0381 (13)
C220.3593 (3)0.9059 (9)0.7142 (2)0.0464 (16)H220.32190.84630.68530.056*C120.2744 (3)1.1173 (8)0.9458 (2)0.0425 (14)H120.23741.17150.91500.051*C230.4072 (3)0.9819 (8)0.7081 (2)0.0457 (16)C110.2759 (3)1.1239 (8)0.9918 (2)0.0445 (15)H110.24161.18440.99250.053*C180.1387 (3)0.5089 (8)0.7500 (3)0.0480 (16)	H16	0.2628	0.6582	0.8673	0.046*
H220.32190.84630.68530.056*C120.2744 (3)1.1173 (8)0.9458 (2)0.0425 (14)H120.23741.17150.91500.051*C230.4072 (3)0.9819 (8)0.7081 (2)0.0457 (16)C110.2759 (3)1.1239 (8)0.9918 (2)0.0445 (15)H110.24161.18440.99250.053*C180.1387 (3)0.5089 (8)0.7500 (3)0.0480 (16)	C22	0.3593 (3)	0.9059 (9)	0.7142 (2)	0.0464 (16)
C120.2744 (3)1.1173 (8)0.9458 (2)0.0425 (14)H120.23741.17150.91500.051*C230.4072 (3)0.9819 (8)0.7081 (2)0.0457 (16)C110.2759 (3)1.1239 (8)0.9918 (2)0.0445 (15)H110.24161.18440.99250.053*C180.1387 (3)0.5089 (8)0.7500 (3)0.0480 (16)	H22	0.3219	0.8463	0.6853	0.056*
H120.23741.17150.91500.051*C230.4072 (3)0.9819 (8)0.7081 (2)0.0457 (16)C110.2759 (3)1.1239 (8)0.9918 (2)0.0445 (15)H110.24161.18440.99250.053*C180.1387 (3)0.5089 (8)0.7500 (3)0.0480 (16)	C12	0.2744 (3)	1.1173 (8)	0.9458 (2)	0.0425 (14)
C230.4072 (3)0.9819 (8)0.7081 (2)0.0457 (16)C110.2759 (3)1.1239 (8)0.9918 (2)0.0445 (15)H110.24161.18440.99250.053*C180.1387 (3)0.5089 (8)0.7500 (3)0.0480 (16)	H12	0.2374	1.1715	0.9150	0.051*
C110.2759 (3)1.1239 (8)0.9918 (2)0.0445 (15)H110.24161.18440.99250.053*C180.1387 (3)0.5089 (8)0.7500 (3)0.0480 (16)	C23	0.4072 (3)	0.9819 (8)	0.7081 (2)	0.0457 (16)
H110.24161.18440.99250.053*C180.1387 (3)0.5089 (8)0.7500 (3)0.0480 (16)	C11	0.2759 (3)	1.1239 (8)	0.9918 (2)	0.0445 (15)
C18 0.1387 (3) 0.5089 (8) 0.7500 (3) 0.0480 (16)	H11	0.2416	1.1844	0.9925	0.053*
	C18	0.1387 (3)	0.5089 (8)	0.7500 (3)	0.0480 (16)

supporting information

H18	0.0976	0.4	437	0.7340	0.058*				
Atomic d	Atomic displacement parameters ($Å^2$)								
	U^{11}	U ²²	U^{33}	U^{12}	U^{13}	U^{23}			
Br1	0.0315 (3)	0.0561 (5)	0.0418 (3)	0.0132 (3)	0.0143 (3)	0.0101 (3)			
Br2	0.0679 (5)	0.0629 (5)	0.0378 (3)	0.0107 (4)	0.0334 (3)	0.0182 (3)			
Col	0.0303 (4)	0.0474 (5)	0.0209 (3)	0.0058 (4)	0.0121 (3)	0.0074 (3)			
02	0.036 (2)	0.052 (3)	0.0194 (16)	0.0137 (19)	0.0118 (15)	0.0036 (16)			
O3	0.034 (2)	0.063 (3)	0.0200 (16)	-0.001(2)	0.0066 (15)	0.0088 (17)			
N2	0.027 (2)	0.031 (3)	0.0247 (19)	0.010 (2)	0.0150 (18)	0.0085 (18)			
N1	0.025 (2)	0.039 (3)	0.0226 (19)	0.010(2)	0.0126 (17)	0.0071 (18)			
N3	0.032 (2)	0.038 (3)	0.0239 (19)	0.002 (2)	0.0144 (18)	0.0046 (19)			
N4	0.026 (2)	0.039 (3)	0.0194 (18)	0.002 (2)	0.0085 (18)	0.0029 (18)			
C41	0.029 (3)	0.055 (4)	0.026 (2)	-0.006(3)	0.017 (2)	-0.002(2)			
C28	0.033 (3)	0.036 (3)	0.033 (3)	0.002 (3)	0.019 (2)	-0.002(2)			
C36	0.047 (3)	0.042 (4)	0.027 (2)	0.005 (3)	0.023 (3)	0.006 (2)			
C40	0.024 (3)	0.027 (3)	0.022 (2)	0.005 (2)	0.010 (2)	0.004 (2)			
C27	0.029 (3)	0.035 (3)	0.017 (2)	0.008 (2)	0.009 (2)	-0.002(2)			
C46	0.023 (3)	0.031 (3)	0.034 (3)	0.005 (2)	0.015 (2)	0.002 (2)			
C45	0.045 (3)	0.061 (5)	0.035 (3)	-0.005(3)	0.029 (3)	-0.007(3)			
C48	0.028 (3)	0.049 (4)	0.022 (2)	-0.002(3)	0.012 (2)	0.001 (2)			
C33	0.031 (3)	0.042 (4)	0.032 (3)	0.009 (3)	0.016 (2)	0.003 (2)			
C49	0.024 (3)	0.043 (4)	0.030 (2)	0.003 (3)	0.013 (2)	0.002 (2)			
C35	0.030 (3)	0.041 (4)	0.021 (2)	0.010 (3)	0.013 (2)	0.002 (2)			
C34	0.030 (3)	0.037 (3)	0.021 (2)	0.004 (2)	0.013 (2)	0.000 (2)			
C43	0.047 (4)	0.050 (4)	0.060 (4)	0.023 (3)	0.036 (3)	0.011 (3)			
C44	0.053 (4)	0.072 (5)	0.055 (4)	-0.002 (4)	0.043 (3)	-0.010 (3)			
C31	0.034 (3)	0.068 (5)	0.067 (4)	0.003 (3)	0.028 (3)	0.003 (4)			
C50	0.042 (3)	0.043 (4)	0.044 (3)	0.001 (3)	0.029 (3)	-0.007(3)			
C47	0.022 (2)	0.029 (3)	0.024 (2)	-0.003 (2)	0.013 (2)	-0.003(2)			
C42	0.033 (3)	0.071 (5)	0.043 (3)	0.006 (3)	0.026 (3)	0.008 (3)			
C37	0.041 (3)	0.049 (4)	0.041 (3)	-0.006(3)	0.021 (3)	0.007 (3)			
C51	0.038 (3)	0.055 (4)	0.024 (2)	0.005 (3)	0.018 (2)	-0.004(2)			
C32	0.031 (3)	0.069 (5)	0.045 (3)	0.005 (3)	0.018 (3)	0.004 (3)			
C39	0.033 (3)	0.039 (4)	0.022 (2)	0.002 (3)	0.013 (2)	0.005 (2)			
C52	0.024 (3)	0.031 (3)	0.026 (2)	-0.001(2)	0.011 (2)	-0.002 (2)			
C29	0.049 (4)	0.048 (4)	0.045 (3)	0.006 (3)	0.027 (3)	0.012 (3)			
C30	0.041 (4)	0.097 (6)	0.063 (4)	0.004 (4)	0.037 (3)	0.020 (4)			
C38	0.033 (3)	0.054 (4)	0.035 (3)	-0.008(3)	0.011 (3)	0.006 (3)			
Br3	0.0629 (5)	0.1340 (9)	0.0506 (4)	0.0121 (5)	0.0425 (4)	-0.0018 (4)			
Br4	0.0482 (4)	0.1339 (8)	0.0419 (3)	0.0164 (4)	0.0321 (3)	0.0144 (4)			
Co2	0.0329 (4)	0.0487 (5)	0.0187 (3)	-0.0001 (4)	0.0099 (3)	-0.0015 (3)			
01	0.036 (2)	0.066 (3)	0.0241 (17)	0.003 (2)	0.0122 (16)	-0.0008 (18)			
04	0.035 (2)	0.061 (3)	0.0247 (17)	-0.005 (2)	0.0129 (16)	-0.0056 (18)			
N6	0.030 (2)	0.047 (3)	0.0204 (19)	-0.006 (2)	0.0116 (18)	-0.0050 (19)			
N5	0.031 (2)	0.038 (3)	0.0220 (19)	-0.002 (2)	0.0120 (18)	-0.0006 (18)			
N7	0.027 (2)	0.046 (3)	0.0221 (19)	0.012 (2)	0.0103 (18)	0.0069 (19)			

N8	0.029 (2)	0.054 (3)	0.0173 (18)	-0.005 (2)	0.0098 (18)	-0.004 (2)
C13	0.030 (3)	0.049 (4)	0.029 (3)	-0.012 (3)	0.014 (2)	-0.010 (2)
C21	0.027 (3)	0.053 (4)	0.025 (2)	0.005 (3)	0.014 (2)	0.001 (2)
C14	0.029 (3)	0.046 (4)	0.022 (2)	0.013 (3)	0.014 (2)	0.003 (2)
C8	0.027 (3)	0.047 (4)	0.029 (2)	-0.014 (3)	0.014 (2)	-0.011 (2)
C3	0.044 (3)	0.051 (4)	0.027 (3)	-0.003 (3)	0.017 (3)	-0.005 (3)
C19	0.032 (3)	0.035 (4)	0.050 (3)	0.001 (3)	0.016 (3)	-0.007 (3)
C6	0.041 (3)	0.050 (4)	0.024 (2)	-0.001 (3)	0.014 (2)	0.007 (2)
C2	0.028 (3)	0.035 (3)	0.022 (2)	-0.005 (3)	0.009 (2)	0.000 (2)
C9	0.037 (3)	0.047 (4)	0.031 (3)	-0.013 (3)	0.019 (2)	-0.006 (2)
C4	0.045 (4)	0.064 (5)	0.038 (3)	0.007 (3)	0.026 (3)	-0.003 (3)
C15	0.034 (3)	0.036 (4)	0.031 (3)	0.019 (3)	0.018 (2)	0.010 (2)
C26	0.031 (3)	0.061 (4)	0.025 (2)	0.006 (3)	0.014 (2)	0.002 (3)
C1	0.028 (3)	0.038 (4)	0.025 (2)	-0.010 (3)	0.012 (2)	-0.006 (2)
C10	0.036 (3)	0.061 (5)	0.042 (3)	-0.013 (3)	0.024 (3)	-0.010 (3)
C17	0.047 (4)	0.031 (4)	0.072 (4)	0.005 (3)	0.039 (3)	0.012 (3)
C20	0.027 (3)	0.021 (3)	0.038 (3)	0.001 (2)	0.016 (2)	-0.003 (2)
C24	0.037 (3)	0.072 (5)	0.057 (4)	-0.003 (3)	0.032 (3)	0.009 (3)
C5	0.037 (3)	0.055 (5)	0.044 (3)	0.009 (3)	0.020 (3)	0.005 (3)
C7	0.028 (3)	0.036 (3)	0.026 (2)	-0.009 (3)	0.015 (2)	-0.004 (2)
C25	0.032 (3)	0.058 (4)	0.038 (3)	-0.017 (3)	0.015 (3)	-0.005 (3)
C16	0.042 (3)	0.031 (3)	0.040 (3)	0.006 (3)	0.023 (3)	0.006 (3)
C22	0.035 (3)	0.073 (5)	0.029 (3)	0.012 (3)	0.018 (3)	0.007 (3)
C12	0.034 (3)	0.044 (4)	0.041 (3)	0.009 (3)	0.017 (3)	0.002 (3)
C23	0.038 (3)	0.068 (5)	0.038 (3)	0.009 (3)	0.026 (3)	0.008 (3)
C11	0.039 (3)	0.047 (4)	0.051 (3)	-0.005 (3)	0.028 (3)	-0.005 (3)
C18	0.032 (3)	0.038 (4)	0.068 (4)	0.004 (3)	0.025 (3)	0.000 (3)

Geometric parameters (Å, °)

Br1-C49	1.904 (5)	Br3—C10	1.889 (6)
Br2—C36	1.898 (5)	Br4—C23	1.893 (6)
Co1—O2	1.912 (4)	Co2—O1	1.930 (4)
Col—O3	1.903 (4)	Co2—O4	1.912 (4)
Co1—N2	1.975 (4)	Co2—N6	1.961 (4)
Co1—N3	1.967 (4)	Co2—N7	1.957 (4)
O2—C52	1.328 (5)	O1—C13	1.322 (6)
O3—C39	1.325 (5)	O4—C26	1.316 (6)
N2-C40	1.339 (6)	N6—C1	1.332 (6)
N2-C41	1.399 (6)	N6—C2	1.388 (7)
N1-C40	1.358 (6)	N5—C1	1.385 (6)
N1-C46	1.390 (6)	N5—C7	1.396 (7)
N1—H1A	0.8600	N5—H5A	0.8600
N3—C27	1.336 (6)	N7—C14	1.330 (6)
N3—C28	1.389 (7)	N7—C15	1.388 (7)
N4—C27	1.366 (6)	N8—C14	1.372 (6)
N4—C33	1.375 (7)	N8—C20	1.384 (7)
N4—H4A	0.8600	N8—H8A	0.8600

$\begin{array}{ccccc} C41-C42 & 1.378 (8) & C13-C12 & 1.400 (8) \\ C41-C46 & 1.392 (7) & C13-C8 & 1.1412 (8) \\ C28-C33 & 1.388 (7) & C21-C22 & 1.408 (7) \\ C28-C32 & 1.406 (8) & C21-C26 & 1.424 (8) \\ C36-C37 & 1.391 (8) & C8-C9 & 1.406 (7) \\ C40-C47 & 1.462 (7) & C8-C1 & 1.447 (8) \\ C27-C34 & 1.448 (7) & C3-C4 & 1.399 (8) \\ C45-C44 & 1.362 (8) & C3-H3 & 0.9300 \\ C45-C44 & 1.350 (7) & C19-C18 & 1.351 (9) \\ C48-C49 & 1.350 (7) & C19-C18 & 1.351 (9) \\ C48-C49 & 1.350 (7) & C19-C10 & 1.382 (8) \\ C38-C32 & 1.381 (8) & C6-C7 & 1.381 (7) \\ C48-C49 & 1.350 (7) & C19-C10 & 1.359 (8) \\ C33-C32 & 1.381 (8) & C6-C7 & 1.381 (7) \\ C45-H43 & 0.9300 & C6-C5 & 1.376 (8) \\ C33-C32 & 1.381 (8) & C6-C7 & 1.381 (7) \\ C45-C39 & 1.410 (7) & C9-H9 & 0.9300 \\ C34-C39 & 1.410 (7) & C9-H9 & 0.9300 \\ C34-C39 & 1.410 (7) & C9-H9 & 0.9300 \\ C43-C42 & 1.385 (8) & C4-C5 & 1.378 (8) \\ C43-C44 & 1.403 (8) & C4-H4 & 0.9300 \\ C43-C44 & 1.403 (8) & C4-H4 & 0.9300 \\ C43-C44 & 1.403 (8) & C4-H4 & 0.9300 \\ C43-C44 & 1.403 (8) & C4-H4 & 0.9300 \\ C15-C16 & 1.399 (7) \\ C44-H44 & 0.9300 & C15-C16 & 1.399 (7) \\ C44-H44 & 0.9300 & C15-C16 & 1.399 (7) \\ C44-H44 & 0.9300 & C15-C16 & 1.399 (7) \\ C44-H44 & 0.9300 & C15-C16 & 1.399 (7) \\ C44-H44 & 0.9300 & C15-C16 & 1.399 (7) \\ C44-H44 & 0.9300 & C15-C16 & 1.399 (7) \\ C44-H44 & 0.9300 & C15-C16 & 1.399 (7) \\ C44-H44 & 0.9300 & C15-C16 & 1.399 (7) \\ C44-H44 & 0.9300 & C15-C16 & 1.399 (7) \\ C44-H44 & 0.9300 & C15-C16 & 1.399 (7) \\ C44-H42 & 0.9300 & C15-C16 & 1.399 (7) \\ C31-C32 & 1.381 (7) & C2-H22 & 0.9300 \\ C31-H31 & 0.9300 & C15-C16 & 1.399 (7) \\ C31-C32 & 1.381 (7) & C2-H24 & 0.9300 \\ C31-H31 & 0.9300 & C15-C16 & 1.399 (7) \\ C31-C32 & 1.381 (7) & C2-H24 & 0.9300 \\ C31-H31 & 0.9300 & C16-H16 & 0.9300 \\ C31-H31 & 0.9300 & C16-H16 & 0.9300 \\ C31-H32 & 0.9300 & C16-H16 & 0.9300 \\ C32-H32 & 0.9300 & C12-H12 & 0.9300 \\ C32-H32 & 0.9300 & C12-H12 & 0.9300 \\ C32-H32 & 0.9300 & C12-H12 & 0.9300 \\ C32-C1-N2 & 1.281 (17) & 04-C2-N6 & 11.360 (17) \\ O3-C01-N2 & 12.81 (17) & 04-C2-N6 & 11.360 (17) \\ O3-C01-N2 & 12.81 (17) & 04-C2-N6 &$				
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C41—C42	1.378 (8)	C13—C12	1.400 (8)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C41—C46	1.392 (7)	C13—C8	1.412 (8)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C28—C33	1.388 (7)	C21—C22	1.408 (7)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C28—C29	1.406 (8)	C21—C26	1.424 (8)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C36—C35	1.334 (8)	C21—C14	1.430 (8)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C36—C37	1 391 (8)	C8—C9	1 406 (7)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C40—C47	1.691(0) 1.462(7)	C8—C1	1 447 (8)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C27 - C34	1.448(7)	C3 - C4	1 369 (8)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C_{46}	1.110(7) 1.377(7)	$C_3 - C_2$	1.309(0) 1.389(7)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C45 - C44	1.377(7) 1.362(8)	C3—C2 C3—H3	0.9300
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$C_{45} = U_{45}$	0.0300	C_{10} C_{18}	1 351 (0)
$\begin{array}{ccccc} C48-C49 & 1.330 (1) & C19-C20 & 1.332 (26) \\ C48-C47 & 1.405 (7) & C19-C19 & 0.9300 \\ C48-H48 & 0.9300 & C6-C5 & 1.376 (8) \\ C33-C32 & 1.381 (8) & C6-C7 & 1.381 (7) \\ C49-C50 & 1.391 (7) & C6-H6 & 0.9300 \\ C35-C34 & 1.414 (6) & C2-C7 & 1.401 (6) \\ C35-H35 & 0.9300 & C9-C10 & 1.359 (8) \\ C34-C39 & 1.410 (7) & C9-H9 & 0.9300 \\ C43-C42 & 1.385 (8) & C4-C5 & 1.378 (8) \\ C43-C44 & 1.403 (8) & C4-H4 & 0.9300 \\ C43-H43 & 0.9300 & C15-C16 & 1.399 (7) \\ C44-H44 & 0.9300 & C15-C20 & 1.403 (7) \\ C31-C32 & 1.386 (9) & C26-C25 & 1.420 (8) \\ C31-C30 & 1.391 (9) & C10-C11 & 1.387 (8) \\ C31-H31 & 0.9300 & C17-C16 & 1.370 (8) \\ C50-L51 & 1.354 (7) & C17-C18 & 1.387 (8) \\ C42-H42 & 0.9300 & C17-H17 & 0.9300 \\ C47-C52 & 1.417 (6) & C24-C25 & 1.361 (8) \\ C42-H42 & 0.9300 & C2-H5 & 0.9300 \\ C51-C52 & 1.383 (7) & C25-H25 & 0.9300 \\ C51-C52 & 1.383 (7) & C25-H25 & 0.9300 \\ C51-C52 & 1.383 (7) & C25-H25 & 0.9300 \\ C51-C52 & 1.383 (7) & C25-H25 & 0.9300 \\ C51-H51 & 0.9300 & C16-H16 & 0.9300 \\ C51-C52 & 1.383 (7) & C25-H25 & 0.9300 \\ C37-H37 & 0.9300 & C24-C23 & 1.351 (9) \\ C37-C38 & 1.375 (8) & C12-C11 & 1.364 (8) \\ C29-H29 & 0.9300 & C16-H16 & 0.9300 \\ C32-H32 & 0.9300 & C16-H16 & 0.9300 \\ C30-H30 & 0.9300 & C16-H16 & 0.9300 \\ C30-H30 & 0.9300 & C18-H18 & 0.9300 \\ C30-H30 & 0.9300 & C18-H18 & 0.9300 \\ C30-H30 & 0.9300 & C18-H18 & 0.9300 \\ C30-C1-N2 & 107.28 (18) & 04-Co2-N7 & 94.49 (17) \\ 03-Co1-N2 & 121.83 (17) & 04-Co2-N7 & 94.49 (17) \\ 02-Co1-N3 & 93.74 (17) & 04-Co2-N7 & 94.49 (17) \\ 02-Co1-N2 & 121.83 (17) & 04-Co2-N6 & 113.60 (17) \\ 03-Co1-N2 & 121.93 (17) & N7-Co2-N6 & 123.0 (2) \\ C52-O2-Co1 & 123.7 (3) & C13-O1-Co2 & 127.3 (4) \\ C32-O2-Co1 & 123.7 (3) & C13-O1-Co2 & 127.3 (4) \\ C32-O2-Co1 & 123.7 (3) & C13-O1-Co2 & 127.3 (4) \\ C32-C1-N2 & 123.7 (3) & C13-O1-Co2 & 127.3 (4) \\ C32-C1-N2 & 123.7 (3) & C13-O1-Co2 & 127.3 (4) \\ C32-C1-N2 & 123.7 (3) & C13-O1-Co2 & 127.3 (4) \\ C32-C1-N2 & 123.7 (3) & C13-O1-Co2 & 127.3 (4) \\ C32-C1-N2 & 123.7 (3) & C13-O1-Co2 & 127.3 (4) \\ C32-C1-N2 & 123.7 (3) & C13-O1-Co2 & 127.3 (4) \\ $	$C_{43} = 1143$	1.250(7)	C19—C18	1.331(9)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C_{40} C_{49} C_{47}	1.550(7)	C19 - C20	1.362 (6)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C48 - C47	1.405 (7)	C19—H19	0.9300
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C48—H48	0.9300	C6—C5	1.376(8)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C33—C32	1.381 (8)	C6C7	1.381 (7)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C49—C50	1.391 (7)	С6—Н6	0.9300
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C35—C34	1.414 (6)	C2—C7	1.401 (6)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	С35—Н35	0.9300	C9—C10	1.359 (8)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C34—C39	1.410(7)	С9—Н9	0.9300
C43—C441.403 (8)C4—H40.9300C43—H430.9300C15—C161.399 (7)C44—H440.9300C15—C201.403 (7)C31—C321.386 (9)C26—C251.420 (8)C31—C301.391 (9)C10—C111.387 (8)C31—H310.9300C17—C161.370 (8)C50—C511.354 (7)C17—C181.385 (9)C50—H500.9300C17—H170.9300C44—H420.9300C24—C251.361 (8)C42—H420.9300C24—C231.391 (9)C37—C381.375 (7)C24—H240.9300C51—C521.383 (7)C25—H50.9300C51—C521.383 (7)C25—H250.9300C51—C521.382 (8)C22—C231.351 (9)C32—H320.9300C16—H160.9300C39—C381.382 (8)C12—C111.364 (8)C29—H290.9300C12—H120.9300C30—H300.9300C11—H110.9300C38—H380.9300C18—H180.9300C38—H380.9300C18—H180.9300C38—C01—N2121.83 (17)O4—Co2—N794.49 (17)O2—Co1—N222.47 (15)O1—Co2—N6113.60 (17)O3—Co1—N2121.93 (17)N7—Co2—N6123.0 (2)C52—O2—Co1123.7 (3)C13—O1—Co2127.3 (4)	C43—C42	1.385 (8)	C4—C5	1.378 (8)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C43—C44	1.403 (8)	C4—H4	0.9300
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C43—H43	0.9300	C15—C16	1.399 (7)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C44—H44	0.9300	C15—C20	1.403 (7)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C31—C32	1.386 (9)	C26—C25	1.420 (8)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C31—C30	1.391 (9)	C10-C11	1.387 (8)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C31—H31	0.9300	C17—C16	1.370 (8)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C50—C51	1.354 (7)	C17—C18	1.385 (9)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	С50—Н50	0.9300	C17—H17	0.9300
C42—H420.9300C24—C231.391 (9)C37—C381.375 (7)C24—H240.9300C37—H370.9300C5—H50.9300C51—C521.383 (7)C25—H250.9300C51—H510.9300C16—H160.9300C32—H320.9300C22—C231.351 (9)C39—C381.382 (8)C22—H220.9300C29—C301.347 (8)C12—C111.364 (8)C29—H290.9300C12—H120.9300C30—H300.9300C11—H110.9300C38—H380.9300C18—H180.9300O3—Co1—O2107.28 (18)O4—Co2—O1125.57 (19)O3—Co1—N393.74 (17)O4—Co2—N794.49 (17)O2—Co1—N3121.01 (17)O1—Co2—N7108.97 (17)O3—Co1—N2121.83 (17)O4—Co2—N6113.60 (17)O2—Co1—N292.47 (15)O1—Co2—N693.86 (17)N3—Co1—N2121.93 (17)N7—Co2—N6123.0 (2)C52—O2—Co1123.7 (3)C13—O1—Co2127.3 (4)	C47—C52	1.417 (6)	C24—C25	1.361 (8)
C37-C38 $1.375(7)$ $C24-H24$ 0.9300 $C37-H37$ 0.9300 $C5-H5$ 0.9300 $C51-C52$ $1.383(7)$ $C25-H25$ 0.9300 $C51-H51$ 0.9300 $C16-H16$ 0.9300 $C32-H32$ 0.9300 $C22-C23$ $1.351(9)$ $C39-C38$ $1.382(8)$ $C22-H22$ 0.9300 $C29-C30$ $1.347(8)$ $C12-C11$ $1.364(8)$ $C29-H29$ 0.9300 $C12-H12$ 0.9300 $C30-H30$ 0.9300 $C12-H12$ 0.9300 $C38-H38$ 0.9300 $C18-H18$ 0.9300 $C38-H38$ 0.9300 $C18-H18$ 0.9300 $C3-Co1-O2$ $107.28(18)$ $O4-Co2-O1$ $125.57(19)$ $O3-Co1-N3$ $93.74(17)$ $O4-Co2-N7$ $94.49(17)$ $O2-Co1-N3$ $121.01(17)$ $O1-Co2-N7$ $108.97(17)$ $O3-Co1-N2$ $121.83(17)$ $O4-Co2-N6$ $113.60(17)$ $O2-Co1-N2$ $92.47(15)$ $O1-Co2-N6$ $93.86(17)$ $N3-Co1-N2$ $121.93(17)$ $N7-Co2-N6$ $123.0(2)$ $C52-O2-Co1$ $123.7(3)$ $C13-O1-Co2$ $127.3(4)$	C42—H42	0.9300	C24—C23	1.391 (9)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C37 - C38	1 375 (7)	C24—H24	0.9300
C51 - L57L5300C51 - L52L5300C51C521.383 (7)C25H250.9300C51H510.9300C16H160.9300C32H320.9300C22C231.351 (9)C39C381.382 (8)C22H220.9300C29C301.347 (8)C12C111.364 (8)C29H290.9300C12H120.9300C30H300.9300C11H110.9300C38H380.9300C18H180.9300O3Co1N393.74 (17)O4Co2N794.49 (17)O2Co1N3121.01 (17)O1Co2N7108.97 (17)O3Co1N2121.83 (17)O4Co2N6113.60 (17)O2Co1N292.47 (15)O1Co2N693.86 (17)N3Co1N2121.93 (17)N7Co2N6123.0 (2)C52O2Co1123.7 (3)C13O1Co2127.3 (4)	C37—H37	0.9300	C5—H5	0.9300
C51C521.365 (1)C251.250.9300C51-H510.9300C16-H160.9300C32-H320.9300C22-C231.351 (9)C39-C381.382 (8)C22-H220.9300C29-C301.347 (8)C12-C111.364 (8)C29-H290.9300C12-H120.9300C30-H300.9300C11-H110.9300C38-H380.9300C18-H180.9300O3-Co1-O2107.28 (18)O4-Co2-O1125.57 (19)O3-Co1-N393.74 (17)O4-Co2-N794.49 (17)O2-Co1-N3121.01 (17)O1-Co2-N7108.97 (17)O3-Co1-N2121.83 (17)O4-Co2-N6113.60 (17)O2-Co1-N292.47 (15)O1-Co2-N693.86 (17)N3-Co1-N2121.93 (17)N7-Co2-N6123.0 (2)C52-O2-Co1123.7 (3)C13-O1-Co2127.3 (4)	$C_{51} - C_{52}$	1.383(7)	C25—H25	0.9300
C31—11310.9300C10—11100.9300C32—H320.9300C22—C231.351 (9)C39—C381.382 (8)C22—H220.9300C29—C301.347 (8)C12—C111.364 (8)C29—H290.9300C12—H120.9300C30—H300.9300C11—H110.9300C38—H380.9300C18—H180.9300O3—Co1—O2107.28 (18)O4—Co2—O1125.57 (19)O3—Co1—N393.74 (17)O4—Co2—N794.49 (17)O2—Co1—N3121.01 (17)O1—Co2—N7108.97 (17)O3—Co1—N2121.83 (17)O4—Co2—N6113.60 (17)O2—Co1—N292.47 (15)O1—Co2—N693.86 (17)N3—Co1—N2121.93 (17)N7—Co2—N6123.0 (2)C52—O2—Co1123.7 (3)C13—O1—Co2127.3 (4)	C51 H51	0.0300	C16 H16	0.9300
$C_{32}=1132$ 0.9300 $C_{22}=C_{23}$ $1.331(9)$ $C_{39}=C_{38}$ $1.382(8)$ $C_{22}=H_{22}$ 0.9300 $C_{29}=C_{30}$ $1.347(8)$ $C_{12}=C_{11}$ $1.364(8)$ $C_{29}=H_{29}$ 0.9300 $C_{12}=H_{12}$ 0.9300 $C_{30}=H_{30}$ 0.9300 $C_{11}=H_{11}$ 0.9300 $C_{38}=H_{38}$ 0.9300 $C_{18}=H_{18}$ 0.9300 $O_{3}=Co_{1}=N_{3}$ $93.74(17)$ $O_{4}=Co_{2}=N7$ $94.49(17)$ $O_{2}=Co_{1}=N_{3}$ $121.01(17)$ $O_{1}=Co_{2}=N7$ $108.97(17)$ $O_{3}=Co_{1}=N_{2}$ $121.83(17)$ $O_{4}=Co_{2}=N6$ $113.60(17)$ $O_{2}=Co_{1}=N_{2}$ $92.47(15)$ $O_{1}=Co_{2}=N6$ $93.86(17)$ $N_{3}=Co_{1}=N_{2}$ $121.93(17)$ $N_{7}=Co_{2}=N6$ $123.0(2)$ $C_{52}=O_{2}=Co_{1}$ $123.7(3)$ $C_{13}=O_{1}=Co_{2}$ $127.3(4)$		0.9300	C10 $C10$ $C10$	1 351 (0)
C39—C38 $1.382 (8)$ $C22 = H22$ 0.9300 C29—C30 $1.347 (8)$ C12—C11 $1.364 (8)$ C29—H29 0.9300 C12—H12 0.9300 C30—H30 0.9300 C11—H11 0.9300 C38—H38 0.9300 C18—H18 0.9300 O3—Co1—O2 $107.28 (18)$ O4—Co2—O1 $125.57 (19)$ O3—Co1—N3 $93.74 (17)$ O4—Co2—N7 $94.49 (17)$ O2—Co1—N3 $121.01 (17)$ O1—Co2—N7 $108.97 (17)$ O3—Co1—N2 $121.83 (17)$ O4—Co2—N6 $113.60 (17)$ O2—Co1—N2 $92.47 (15)$ O1—Co2—N6 $93.86 (17)$ N3—Co1—N2 $121.93 (17)$ N7—Co2—N6 $123.0 (2)$ C52—O2—Co1 $123.7 (3)$ C13—O1—Co2 $127.3 (4)$	C_{32} C_{30} C_{38}	1 2 9 2 (9)	$C_{22} = C_{23}$	0.0200
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$C_{20} = C_{20}$	1.362(6) 1.247(8)	C_{22} $-H_{22}$	0.9300
C29—H29 0.9300 $C12$ —H12 0.9300 $C30$ —H30 0.9300 $C11$ —H11 0.9300 $C38$ —H38 0.9300 $C18$ —H18 0.9300 $O3$ —Co1—O2 $107.28 (18)$ $O4$ —Co2—O1 $125.57 (19)$ $O3$ —Co1—N3 $93.74 (17)$ $O4$ —Co2—N7 $94.49 (17)$ $O2$ —Co1—N3 $121.01 (17)$ $O1$ —Co2—N7 $108.97 (17)$ $O3$ —Co1—N2 $121.83 (17)$ $O4$ —Co2—N6 $113.60 (17)$ $O2$ —Co1—N2 $92.47 (15)$ $O1$ —Co2—N6 $93.86 (17)$ $N3$ —Co1—N2 $121.93 (17)$ $N7$ —Co2—N6 $123.0 (2)$ $C52$ —O2—Co1 $123.7 (3)$ $C13$ —O1—Co2 $127.3 (4)$	$C_{29} = C_{30}$	1.347 (8)		1.304 (8)
C30—H30 0.9300 $C11$ —H11 0.9300 C38—H38 0.9300 $C18$ —H18 0.9300 O3—Co1—O2 $107.28 (18)$ $O4$ —Co2—O1 $125.57 (19)$ O3—Co1—N3 $93.74 (17)$ $O4$ —Co2—N7 $94.49 (17)$ O2—Co1—N3 $121.01 (17)$ $O1$ —Co2—N7 $108.97 (17)$ O3—Co1—N2 $121.83 (17)$ $O4$ —Co2—N6 $113.60 (17)$ O2—Co1—N2 $92.47 (15)$ $O1$ —Co2—N6 $93.86 (17)$ N3—Co1—N2 $121.93 (17)$ N7—Co2—N6 $123.0 (2)$ C52—O2—Co1 $123.7 (3)$ $C13$ —O1—Co2 $127.3 (4)$	C29—H29	0.9300	C12—H12	0.9300
C38—H38 0.9300 C18—H18 0.9300 O3—Co1—O2 107.28 (18) O4—Co2—O1 125.57 (19) O3—Co1—N3 93.74 (17) O4—Co2—N7 94.49 (17) O2—Co1—N3 121.01 (17) O1—Co2—N7 108.97 (17) O3—Co1—N2 121.83 (17) O4—Co2—N6 113.60 (17) O2—Co1—N2 92.47 (15) O1—Co2—N6 93.86 (17) N3—Co1—N2 121.93 (17) N7—Co2—N6 123.0 (2) C52—O2—Co1 123.7 (3) C13—O1—Co2 127.3 (4)	C30—H30	0.9300	CII—HII	0.9300
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	С38—Н38	0.9300	C18—H18	0.9300
O3—Co1—N393.74 (17)O4—Co2—N794.49 (17)O2—Co1—N3121.01 (17)O1—Co2—N7108.97 (17)O3—Co1—N2121.83 (17)O4—Co2—N6113.60 (17)O2—Co1—N292.47 (15)O1—Co2—N693.86 (17)N3—Co1—N2121.93 (17)N7—Co2—N6123.0 (2)C52—O2—Co1123.7 (3)C13—O1—Co2127.3 (4)	O3—Co1—O2	107.28 (18)	O4—Co2—O1	125.57 (19)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O3—Co1—N3	93.74 (17)	O4—Co2—N7	94.49 (17)
O3—Co1—N2121.83 (17)O4—Co2—N6113.60 (17)O2—Co1—N292.47 (15)O1—Co2—N693.86 (17)N3—Co1—N2121.93 (17)N7—Co2—N6123.0 (2)C52—O2—Co1123.7 (3)C13—O1—Co2127.3 (4)	O2—Co1—N3	121.01 (17)	O1—Co2—N7	108.97 (17)
O2-Co1-N292.47 (15)O1-Co2-N693.86 (17)N3-Co1-N2121.93 (17)N7-Co2-N6123.0 (2)C52-O2-Co1123.7 (3)C13-O1-Co2127.3 (4)	O3—Co1—N2	121.83 (17)	O4—Co2—N6	113.60 (17)
N3—Co1—N2121.93 (17)N7—Co2—N6123.0 (2)C52—O2—Co1123.7 (3)C13—O1—Co2127.3 (4)	O2—Co1—N2	92.47 (15)	O1—Co2—N6	93.86 (17)
C52—O2—Co1 123.7 (3) C13—O1—Co2 127.3 (4)	N3—Co1—N2	121.93 (17)	N7—Co2—N6	123.0 (2)
	C52—O2—Co1	123.7 (3)	C13—O1—Co2	127.3 (4)

C39-O3-Co1	125 5 (3)	C26-04-Co2	126 5 (4)
$C40 - N^2 - C41$	106.9 (4)	C1 - N6 - C2	107.9(4)
C40 - N2 - Co1	1214(3)	$C1 - N6 - Co^2$	1240(4)
$C_{41} = N_{2} = C_{01}$	121.1(3) 1304(3)	$C_2 = N_6 = C_0^2$	127.7(3)
C_{40} N1 C_{46}	108.6(4)	C1 N5 C7	127.7(3)
C40 N1 H1A	108.0 (4)	C1 = N5 = H5A	109.5 (4)
C46 N1 U1A	125.7	C7 N5 U5 A	125.5
C40— $N1$ — $H1A$	123.7	$C_{-N} = H_{J} = H_{J}$	123.3
$C_2/-N_3-C_{28}$	106.7 (4)	C14 N7 C15	107.2 (4)
$C_2/-N_3$ -Col	121.0 (4)	C14 - N / - C02	123.4 (4)
C28—N3—C01	131.4 (3)	C15 - N / - C02	128.2 (3)
C27—N4—C33	109.1 (4)	C14—N8—C20	109.3 (4)
C27—N4—H4A	125.4	C14—N8—H8A	125.4
C33—N4—H4A	125.4	C20—N8—H8A	125.4
C42—C41—C46	121.4 (5)	O1—C13—C12	117.4 (5)
C42—C41—N2	130.0 (5)	O1—C13—C8	125.4 (5)
C46—C41—N2	108.6 (5)	C12—C13—C8	117.2 (5)
C33—C28—N3	109.2 (5)	C22—C21—C26	118.3 (5)
C33—C28—C29	119.2 (5)	C22—C21—C14	119.4 (5)
N3—C28—C29	131.5 (5)	C26—C21—C14	122.3 (5)
C35—C36—C37	121.1 (5)	N7—C14—N8	109.7 (5)
C35—C36—Br2	121.3 (4)	N7—C14—C21	126.3 (5)
C37—C36—Br2	117.6 (4)	N8—C14—C21	124.0 (4)
N2-C40-N1	110.3 (4)	C9—C8—C13	119.0 (5)
N2-C40-C47	125.4 (4)	C9—C8—C1	118.7 (5)
N1-C40-C47	124.3 (4)	C13 - C8 - C1	122.3(5)
N3-C27-N4	109.6 (5)	C4-C3-C2	1181(5)
N3-C27-C34	126.6(4)	C4—C3—H3	121.0
N4_C27_C34	123.9(4)	C2_C3_H3	121.0
C45 - C46 - N1	132.6 (5)	C_{18} C_{19} C_{20}	115.6 (6)
$C_{45} = C_{46} = C_{41}$	132.0(5)	$C_{18} = C_{19} = C_{20}$	113.0 (0)
$C_{45} - C_{40} - C_{41}$	121.7(3) 105.7(4)	$C_{10} = C_{10} = H_{10}$	122.2
$\begin{array}{cccc} \mathbf{N} & -\mathbf{C} 4 0 & -\mathbf{C} 4 1 \\ \mathbf{C} 4 4 & \mathbf{C} 4 5 & \mathbf{C} 4 6 \end{array}$	103.7(4)	C20-C19-H19	122.2
$C_{44} = C_{45} = C_{40}$	110.9 (3)	$C_{5} = C_{6} = C_{7}$	113.8 (3)
C44—C45—H45	121.5		122.1
C46—C45—H45	121.5	C/-C6-H6	122.1
C49—C48—C47	120.8 (4)	N6-C2-C3	130.6 (4)
C49—C48—H48	119.6	N6—C2—C7	109.7 (4)
C47—C48—H48	119.6	C3—C2—C7	119.7 (5)
N4—C33—C32	132.0 (5)	C10—C9—C8	121.5 (6)
N4—C33—C28	105.2 (5)	С10—С9—Н9	119.2
C32—C33—C28	122.7 (6)	С8—С9—Н9	119.2
C48—C49—C50	120.9 (5)	C3—C4—C5	121.0 (6)
C48—C49—Br1	121.1 (4)	C3—C4—H4	119.5
C50—C49—Br1	118.0 (4)	С5—С4—Н4	119.5
C36—C35—C34	121.7 (5)	N7—C15—C16	132.2 (5)
С36—С35—Н35	119.2	N7—C15—C20	109.4 (5)
С34—С35—Н35	119.2	C16—C15—C20	118.4 (5)
C39—C34—C35	118.1 (5)	O4—C26—C25	117.2 (5)
C39—C34—C27	122.7 (4)	O4—C26—C21	125.6 (5)

C35—C34—C27	119.1 (4)	C25—C26—C21	117.2 (5)
C42—C43—C44	120.6 (6)	N6-C1-N5	108.8 (5)
C42—C43—H43	119.7	N6-C1-C8	126.7 (5)
C44—C43—H43	119.7	N5-C1-C8	124.5 (4)
C45—C44—C43	122.3 (5)	C9—C10—C11	120.1 (5)
C45—C44—H44	118.9	C9—C10—Br3	119.9 (5)
C43—C44—H44	118.9	C11—C10—Br3	119.8 (5)
C32—C31—C30	121.9 (6)	C16—C17—C18	119.6 (6)
С32—С31—Н31	119.1	С16—С17—Н17	120.2
С30—С31—Н31	119.1	C18—C17—H17	120.2
C51—C50—C49	119.2 (5)	C19—C20—N8	132.4 (5)
С51—С50—Н50	120.4	C19—C20—C15	123.1 (5)
С49—С50—Н50	120.4	N8—C20—C15	104.5 (4)
C48—C47—C52	118.3 (4)	C25—C24—C23	119.4 (6)
C48—C47—C40	119.1 (4)	C25—C24—H24	120.3
C52—C47—C40	122.5 (4)	C23—C24—H24	120.3
C41—C42—C43	117.1 (5)	C6—C5—C4	123.0 (6)
C41—C42—H42	121.5	С6—С5—Н5	118.5
C43—C42—H42	121.5	C4—C5—H5	118.5
C38—C37—C36	118.0 (6)	C6—C7—N5	133.4 (4)
С38—С37—Н37	121.0	C6—C7—C2	122.5 (5)
С36—С37—Н37	121.0	N5—C7—C2	104.1 (4)
C50—C51—C52	122.2 (5)	C24—C25—C26	122.5 (6)
C50—C51—H51	118.9	C24—C25—H25	118.7
C52—C51—H51	118.9	C26—C25—H25	118.7
C33—C32—C31	116.2 (6)	C17—C16—C15	119.0 (5)
С33—С32—Н32	121.9	C17—C16—H16	120.5
С31—С32—Н32	121.9	C15—C16—H16	120.5
O3—C39—C38	117.6 (5)	C23—C22—C21	122.3 (6)
O3—C39—C34	124.3 (5)	C23—C22—H22	118.8
C38—C39—C34	118.1 (4)	C21—C22—H22	118.8
O2—C52—C51	117.5 (4)	C11—C12—C13	123.0 (5)
O2—C52—C47	124.0 (5)	C11—C12—H12	118.5
C51—C52—C47	118.5 (4)	C13—C12—H12	118.5
C30—C29—C28	118.7 (6)	C22—C23—C24	120.3 (6)
С30—С29—Н29	120.7	C22—C23—Br4	120.3 (5)
С28—С29—Н29	120.7	C24—C23—Br4	119.4 (5)
C29—C30—C31	121.2 (6)	C12—C11—C10	119.1 (6)
С29—С30—Н30	119.4	C12—C11—H11	120.4
C31—C30—H30	119.4	C10—C11—H11	120.4
C37—C38—C39	123.0 (5)	C19—C18—C17	124.3 (6)
C37—C38—H38	118.5	C19—C18—H18	117.8
С39—С38—Н38	118.5	C17—C18—H18	117.8

Hydrogen-bond geometry (Å, °)

D—H···A	<i>D</i> —Н	H···A	D····A	<i>D</i> —H··· <i>A</i>
N1—H1A····O1 ⁱ	0.86	2.19	2.895 (5)	139

supporting information

N4—H4A···O2 ⁱⁱ	0.86	2.09	2.849 (5)	147	
N5—H5A···O4 ⁱⁱⁱ	0.86	2.41	3.066 (5)	133	
N8—H8A···O3 ^{iv}	0.86	2.17	2.808 (5)	131	
C4— $H4$ ···Br4 ⁱ	0.93	2.88	3.703 (6)	149	
C6—H6···Br1 ^v	0.93	2.91	3.685 (6)	142	
C35—H35…O2 ⁱⁱ	0.93	2.54	3.394 (7)	153	

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