metal-organic compounds

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Aqua(5,10,15,20-tetraphenylporphyrinato- $\kappa^4 N$)cadmium(II)–18-crown-6 (1/1)

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Key indicators: single-crystal X-ray study; T = 173 K; mean σ (C–C) = 0.003 Å; R factor = 0.028; wR factor = 0.074; data-to-parameter ratio = 16.2.

The title compound, $[Cd(C_{44}H_{28}N_4)(H_2O)]\cdot(C_{12}H_{24}O_6)$, was made by the reaction of the [Cd(TPP)] with an excess of 18crown-6 in chlorobenzene (where TPP is tetraphenylporphyrinate). The Cd^{II} cation is chelated by a TPP anion and coordinated by a water molecule in a distorted N₄O square-pyramidal geometry, the Cd^{II} cation being displaced by 0.7533 (9) Å from the mean plane of four N atoms of TPP anion. The porphyrin core presents a significant distortion, the maximum atomic deviation from the 24-atom mean plane is 0.1517 (2) Å. The 18-crown-6 molecule is linked with the Cd^{II} complex *via* classical O–H···O hydrogen bonds. In the crystal, weak C–H··· π interactions link the complex and 18crown-6 molecules into a three-dimensional supramolecular architecture.

Related literature

For the synthesis, see: Rodesiler *et al.* (1985*b*). For related structures, see: Byrn *et al.* (1991); Ezzayani *et al.* (2013); Rodesiler *et al.* (1985*a*); Mansour *et al.* (2010); Yang *et al.* (2003); Maldonado *et al.* (2009). For bond lengths in Cd^{II} complexes, see: Allen (2002). For further details of geometric distortions in related compounds, see: Scheidt & Lee (1987); Jentzen *et al.* (1997).



Experimental

Crystal data

 $\begin{bmatrix} Cd(C_{44}H_{28}N_4)(H_2O) \end{bmatrix} \cdot C_{12}H_{24}O_6 \\ M_r = 1007.42 \\ Monoclinic, P2_1/n \\ a = 17.1956 (2) Å \\ b = 17.0918 (2) Å \\ c = 17.3903 (2) Å \\ \beta = 106.416 (1)^{\circ} \end{bmatrix}$

Data collection

Agilent Xcalibur (Eos, Gemini ultra) diffractometer Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012) *T*_{min} = 0.959, *T*_{max} = 1.000

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.028$ $wR(F^2) = 0.074$ S = 1.0410009 reflections 619 parameters 2 restraints Z = 4 Mo K α radiation μ = 0.50 mm⁻¹ T = 173 K 0.48 × 0.40 × 0.30 mm

 $V = 4902.72 (10) \text{ Å}^3$

53048 measured reflections 10009 independent reflections 8403 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.027$

H atoms treated by a mixture of independent and constrained refinement $\Delta \rho_{max} = 0.64 \text{ e } \text{\AA}^{-3}$ $\Delta \rho_{min} = -0.53 \text{ e } \text{\AA}^{-3}$

Table 1

Selected bond lengths (Å).

Cd-N1	2.2296 (15)	Cd-N4	2.2265 (15)
Cd-N2	2.2296 (15)	Cd-O1	2.2368 (18)
Cd-N3	2.2322 (16)		

Table 2

Hydrogen-bond geometry (Å, °).

Cg2, Cg3, Cg4 and Cg11 are the centroids of the N2/C6–C9, N3/C11–C14, N4/C16–C19 and C33–C38 rings, respectively.

$D - H \cdot \cdot \cdot A$	D-H	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - \mathbf{H} \cdots A$
01-H101···O4	1.01 (2)	2.06 (2)	3.057 (2)	176
O1−H2 <i>O</i> 1···O6	1.00 (2)	2.04 (2)	3.013 (2)	165
$C31 - H31 \cdots Cg3^{i}$	0.95	2.93	3.651 (2)	133
$C41 - H41 \cdots Cg11^{ii}$	0.95	2.91	3.794 (2)	154
$C44 - H44 \cdots Cg2^{iii}$	0.95	2.95	3.648 (2)	131
$C47 - H47A \cdots Cg2$	0.99	2.91	3.898 (3)	173
$C54-H54B\cdots Cg4$	0.99	2.98	3.971 (3)	176
Symmetry codes: $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{1}{2}.$	(i) $-x + \frac{1}{2}, \frac{1}{2}$	$y - \frac{1}{2}, -z + \frac{1}{2};$	(ii) $-x, -y - x$	+1, -z; (iii)

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996) and *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5709).

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supporting information

Acta Cryst. (2013). E69, m354–m355 [https://doi.org/10.1107/S160053681301489X] Aqua(5,10,15,20-tetraphenylporphyrinato-κ⁴N)cadmium(II)–18-crown-6 (1/1) Hamza Toumi, Yassine Belghith, Jean-Claude Daran and Habib Nasri

S1. Comment

In continuation of our research on the crystal structures of porphyrin complexes in general and the structures of metalloporphyrins resulting from the reaction of these species with the ether crown 18-crown-6 (Mansour *et al.*, 2010; Ezzayani *et al.*, 2013) we herein report the synthesis and crystal structure of the aqua-cadmium tetraphenylporhyrin derivative $[Cd^{II}(TPP)(H_2O)].(18-C-6)$. The coordination geometry of the Cd^{2+} ion is square pyramidal with four Cd— *N*(pyrrole) bonds in the equatorial porphyrin plane and the Cd—O bond with a water axial ligand molecule.

The axial Cd—O(H₂O) bond length [2.237 (2) Å] is within the range [2.210 (2) - 2.326 (1) Å] found for several cadmium-aqua non-porphyrin complexes (CSD refcodes BUYWIB10; Rodesiler *et al.*, 1985*a* and BOQQEE; Maldonado *et al.*, 2009) (CDS, version 5.34, Allen, 2002).

The average equatorial cadmium-pyrrole N atoms distance $(Cd-N_p)$ [2.230 (2) Å] is in the range [2.126 (9) - 2.3167 (3) Å] for Cd(II) porphyrin complexes (CSD refcodes JIVROV; Byrn *et al.*, 1991 and EXACOV; Yang *et al.*, 2003).

The cadmium atom is displaced by 0.8025 (4) Å from the 24 atoms mean plane. The porphyrin core presents a major doming deformation as seen by the positions of the N atoms above the CdN_4C_{20} mean plane (Fig.1) ((Scheidt & Lee, 1987). This is confirmed by the Normal Structural Decomposition (NSD) calculations (Jentzen *et al.*, 1997) with a doming percentage of 47%. These calculations indicated also a saddling and ruffling distortions of the porphyrin core (~ 27% and ~ 14% respectively).

The crystal packing in the *a* and *b* directions assemble to a linear chains linked together by weak C—H $\cdots\pi$ interactions incorporating pyrrole or phenyl rings (Table 1). The parallel chains are sustained together by weak intermolecular hydrogen bonds between the O1 oxygen of the water axial ligand and the oxygene atoms of the 18-crown-6 ether crown molecule (Fig.2).

S2. Experimental

To a solution of [Cd(TPP)] (Rodesiler *et al.* 1985*b*) (20 mg, 0.027 mmol) in chlorobenzene (15 ml) was added an excess of 18-crown-6 (80 mg, 0.300 mmol). The reaction mixture was stirred at room temperature and at the end of the reaction, the color of the solution gradually changes from dark green to blue – purple. The resulting material was crystallized by diffusion of hexanes through the chlorobenzene solution which yields $[Cd(TPP)(H_2O)].(18-C-6)$. The water molecule coordinated to the cadmium come from the hygroscopic 18-crown-6 reagent used in excess.

S3. Refinement

All H atoms attached to C atoms were fixed geometrically and treated as riding with C—H = 0.99 Å (methylene) and 0.95 Å (aromatic) with $U_{iso}(H) = 1.2U_{eq}(C_{aromatic, methylene})$. The two H atoms of the water axial ligand were found in the difference Fourier map and were included in the refinement with $U_{iso}(H) = 1.2U_{eq}(O)$.



Figure 1

An *ORTEP* view of the molecular structure of the title molecule with the atom-numbering. Displacement ellipsoids are drawn at 45%. Except the two H atoms of the water axial ligand, the other H atoms have been omitted for clarity.





Drawing showing the packing in lattice of $[Cd^{II}(TPP)(H_2O)].(18-C-6)$, viewed down the *b* axis.

Aqua(5,10,15,20-tetraphenylporphyrinato- $\kappa^4 N$)cadmium–18-crown-6 (1/1)

Crystal data

 $[Cd(C_{44}H_{28}N_4)(H_2O)] \cdot C_{12}H_{24}O_6$ $M_r = 1007.42$ Monoclinic, $P2_1/n$ Hall symbol: -P 2yn a = 17.1956 (2) Å b = 17.0918 (2) Å c = 17.3903 (2) Å $\beta = 106.416$ (1)° V = 4902.72 (10) Å³ Z = 4

Data collection

Agilent Xcalibur (Eos, Gemini ultra) diffractometer Radiation source: Enhance (Mo) X-ray Source Graphite monochromator Detector resolution: 16.1978 pixels mm⁻¹ ω scans Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012) $T_{\min} = 0.959, T_{\max} = 1.000$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier
Least-squares matrix: full	map
$R[F^2 > 2\sigma(F^2)] = 0.028$	Hydrogen site location: inferred from
$wR(F^2) = 0.074$	neighbouring sites
S = 1.04	H atoms treated by a mixture of independent
10009 reflections	and constrained refinement
619 parameters	$w = 1/[\sigma^2(F_o^2) + (0.0294P)^2 + 3.9972P]$
2 restraints	where $P = (F_o^2 + 2F_c^2)/3$
Primary atom site location: structure-invariant	$(\Delta/\sigma)_{\rm max} = 0.001$
direct methods	$\Delta ho_{ m max} = 0.64 \ { m e} \ { m \AA}^{-3}$
	$\Delta \rho_{\rm min} = -0.53 \text{ e} \text{ Å}^{-3}$

Special details

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

F(000) = 2088

 $\theta = 3.0-30.2^{\circ}$ $\mu = 0.50 \text{ mm}^{-1}$

T = 173 K

 $R_{\rm int} = 0.027$

 $h = -21 \rightarrow 21$

 $k = -21 \rightarrow 21$

 $l = -20 \rightarrow 21$

 $D_{\rm x} = 1.365 {\rm Mg} {\rm m}^{-3}$

Prism. dark purple

 $0.48 \times 0.40 \times 0.30 \text{ mm}$

53048 measured reflections 10009 independent reflections

 $\theta_{\text{max}} = 26.4^{\circ}, \ \theta_{\text{min}} = 3.2^{\circ}$

8403 reflections with $I > 2\sigma(I)$

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å Cell parameters from 20195 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 (\hat{A}^2)

	x	у	Ζ	$U_{ m iso}$ */ $U_{ m eq}$	
Cd	0.265537 (8)	0.245868 (8)	0.053198 (8)	0.02100 (5)	
N1	0.37977 (9)	0.17811 (9)	0.10136 (9)	0.0212 (3)	

N2	0.21008 (9)	0.14476 (9)	0.09930 (9)	0.0214 (3)
N3	0.17605 (9)	0.31526 (9)	0.09616 (10)	0.0231 (3)
N4	0.34586 (9)	0.34841 (9)	0.09638 (9)	0.0220 (3)
01	0.21234 (11)	0.24774 (10)	-0.07997 (11)	0.0422 (4)
O2	0.33082 (9)	0.14168 (9)	-0.11786 (9)	0.0364 (4)
03	0.16534 (9)	0.08322 (9)	-0.15578 (9)	0.0352 (3)
O4	0.03786 (9)	0.18817 (9)	-0.13841 (9)	0.0361 (4)
05	0.06271 (10)	0.34754 (9)	-0.17462 (9)	0.0371 (4)
O6	0.22338 (10)	0.41108 (10)	-0.14125 (10)	0.0444 (4)
07	0.34991 (9)	0.30153 (9)	-0.15312 (8)	0.0322 (3)
C1	0.45563 (11)	0.20529 (11)	0.10492 (11)	0.0211 (4)
C2	0.50969 (12)	0.13908 (11)	0.11073 (12)	0.0271 (4)
H2	0.5655	0.1412	0.1131	0.033*
C3	0.46583 (12)	0.07371 (12)	0.11217 (12)	0.0271 (4)
Н3	0.4853	0.0214	0.1164	0.033*
C4	0.38352 (11)	0.09828 (11)	0.10614 (11)	0.0216 (4)
C5	0.31917 (11)	0.04744 (11)	0.10855 (11)	0.0218 (4)
C6	0.23883 (11)	0.06961 (11)	0.10652 (11)	0.0213 (4)
C7	0.17416 (12)	0.01738 (11)	0.11131 (12)	0.0248 (4)
H7	0.1775	-0.0379	0.1164	0.030*
C8	0.10785 (12)	0.06195 (11)	0.10721 (12)	0.0248 (4)
H8	0.0562	0.0437	0.1089	0.030*
C9	0.13056 (11)	0.14254 (11)	0.09982 (11)	0.0216 (4)
C10	0.07981 (11)	0.20806 (11)	0.09666 (11)	0.0222 (4)
C11	0.10115 (11)	0.28804 (11)	0.09593 (11)	0.0225 (4)
C12	0.04866 (12)	0.35440 (12)	0.09641 (12)	0.0269 (4)
H12	-0.0066	0.3522	0.0961	0.032*
C13	0.09299 (12)	0.41978 (12)	0.09745 (12)	0.0267 (4)
H13	0.0748	0.4722	0.0982	0.032*
C14	0.17375 (11)	0.39514 (11)	0.09725 (11)	0.0225 (4)
C15	0.23970 (11)	0.44530 (11)	0.10023 (11)	0.0225 (4)
C16	0.31955 (11)	0.42321 (11)	0.10184 (11)	0.0225 (4)
C17	0.38757 (12)	0.47598 (12)	0.11154 (12)	0.0277 (4)
H17	0.3862	0.5313	0.1162	0.033*
C18	0.45337 (12)	0.43202 (11)	0.11275 (12)	0.0266 (4)
H18	0.5068	0.4507	0.1187	0.032*
C19	0.42720 (11)	0.35104 (11)	0.10322 (11)	0.0223 (4)
C20	0.47778 (11)	0.28538 (11)	0.10535 (11)	0.0209 (4)
C21	0.56510 (11)	0.30243 (11)	0.11270 (11)	0.0222 (4)
C22	0.58749 (12)	0.34409 (12)	0.05328 (12)	0.0279 (4)
H22	0.5468	0.3618	0.0074	0.034*
C23	0.66821 (13)	0.35997 (12)	0.06010 (13)	0.0317 (5)
H23	0.6825	0.3885	0.0192	0.038*
C24	0.72800 (12)	0.33410 (12)	0.12661 (14)	0.0324 (5)
H24	0.7834	0.3442	0.1311	0.039*
C25	0.70675 (12)	0.29358 (13)	0.18647 (13)	0.0313 (5)
H25	0.7477	0.2763	0.2323	0.038*
C26	0.62602 (12)	0.27795 (12)	0.18002 (12)	0.0258 (4)

H26	0.6121	0.2504	0.2217	0.031*
C27	0.33764 (11)	-0.03828 (11)	0.11456 (12)	0.0229 (4)
C28	0.35747 (12)	-0.07837(12)	0.05283 (12)	0.0269 (4)
H28	0.3607	-0.0504	0.0066	0.032*
C29	0.37260 (12)	-0.15827(12)	0.05755 (14)	0.0322 (5)
H29	0.3859	-0.1846	0.0148	0.039*
C30	0.36830 (13)	-0.19942(12)	0.12482 (15)	0.0353 (5)
H30	0.3777	-0.2543	0.1279	0.042*
C31	0.35036 (14)	-0.16063(13)	0.18735 (14)	0.0376(5)
H31	0 3484	-0.1887	0 2339	0.045*
C32	0.33515(13)	-0.08089(12)	0.18251 (13)	0.0319(5)
H32	0.3229	-0.0548	0.2259	0.0319 (5)
C33	-0.00569(11)	0.19123 (11)	0.2239 0.09717 (11)	0.020(4)
C34	-0.06227(12)	0.19123(11) 0.16238(12)	0.02939(12)	0.0220(4) 0.0267(4)
H34	-0.0462	0.1514	-0.0175	0.0207 (4)
C35	-0.14237(12)	0.1314 0.14041 (12)	0.0175 0.02041 (13)	0.032
U35	-0.1805	0.14941(12) 0.1206	-0.0173	0.0298 (4)
1155 C26	0.1603	0.1230	0.0173	0.030°
C30	-0.10022(12)	0.10322 (11)	0.09690 (15)	0.0294 (4)
П30 С27	-0.2211	0.1370	0.0903	0.035
C37	-0.11035 (13)	0.19221 (14)	0.16515 (14)	0.0359 (5)
H3/	-0.1204	0.2016	0.2125	0.043*
C38	-0.03095 (13)	0.20565 (14)	0.16522 (13)	0.0333 (5)
H38	0.0069	0.2250	0.2123	0.040*
C39	0.22450 (11)	0.53120 (11)	0.10536 (12)	0.0227 (4)
C40	0.18189 (12)	0.57321 (12)	0.03822 (13)	0.0290 (4)
H40	0.1609	0.5470	-0.0115	0.035*
C41	0.16974 (13)	0.65313 (12)	0.04310 (14)	0.0327 (5)
H41	0.1409	0.6812	-0.0034	0.039*
C42	0.19919 (13)	0.69193 (12)	0.11491 (14)	0.0322 (5)
H42	0.1910	0.7467	0.1180	0.039*
C43	0.24083 (15)	0.65080 (13)	0.18261 (14)	0.0385 (5)
H43	0.2606	0.6771	0.2324	0.046*
C44	0.25354 (14)	0.57107 (13)	0.17745 (13)	0.0348 (5)
H44	0.2826	0.5432	0.2240	0.042*
C45	0.30525 (15)	0.06615 (13)	-0.14746 (15)	0.0386 (5)
H45A	0.3508	0.0288	-0.1298	0.046*
H45B	0.2878	0.0669	-0.2068	0.046*
C46	0.23605 (15)	0.04059 (13)	-0.11659 (14)	0.0386 (5)
H46A	0.2261	-0.0161	-0.1265	0.046*
H46B	0.2499	0.0497	-0.0581	0.046*
C47	0.09835 (15)	0.06200 (14)	-0.12725 (15)	0.0410 (6)
H47A	0.1121	0.0705	-0.0686	0.049*
H47B	0.0855	0.0059	-0.1381	0.049*
C48	0.02653 (15)	0.11097 (14)	-0.16878 (15)	0.0402 (5)
H48A	0.0200	0.1115	-0.2272	0.048*
H48B	-0.0232	0.0884	-0.1598	0.048*
C49	-0.02503 (14)	0.23930 (14)	-0.18003 (15)	0.0381 (5)
H49A	-0.0770	0.2231	-0.1711	0.046*

H49B	-0.0309	0.2369	-0.2383	0.046*
C50	-0.00474 (15)	0.32122 (15)	-0.15018 (16)	0.0432 (6)
H50A	-0.0518	0.3560	-0.1724	0.052*
H50B	0.0084	0.3224	-0.0910	0.052*
C51	0.08384 (17)	0.42528 (14)	-0.15134 (18)	0.0485 (6)
H51A	0.1002	0.4292	-0.0921	0.058*
H51B	0.0365	0.4599	-0.1727	0.058*
C52	0.15181 (17)	0.45058 (15)	-0.18254 (17)	0.0482 (6)
H52A	0.1387	0.4389	-0.2406	0.058*
H52B	0.1599	0.5078	-0.1753	0.058*
C53	0.29070 (16)	0.42850 (14)	-0.17172 (16)	0.0449 (6)
H53A	0.3041	0.4849	-0.1646	0.054*
H53B	0.2764	0.4163	-0.2297	0.054*
C54	0.36231 (15)	0.38056 (14)	-0.12745 (15)	0.0416 (6)
H54A	0.4121	0.4011	-0.1381	0.050*
H54B	0.3692	0.3838	-0.0691	0.050*
C55	0.41553 (14)	0.25217 (14)	-0.11332 (14)	0.0374 (5)
H55A	0.4234	0.2542	-0.0547	0.045*
H55B	0.4660	0.2704	-0.1242	0.045*
C56	0.39737 (13)	0.16979 (14)	-0.14272 (14)	0.0381 (5)
H56A	0.3841	0.1685	-0.2019	0.046*
H56B	0.4454	0.1362	-0.1205	0.046*
H1O1	0.1543 (7)	0.2301 (14)	-0.0972 (15)	0.046*
H2O1	0.2057 (15)	0.3017 (8)	-0.1024 (14)	0.046*

Atomic displacement parameters $(Å^2)$

U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
0.01691 (8)	0.02131 (8)	0.02469 (8)	-0.00051 (5)	0.00575 (5)	0.00129 (5)
0.0182 (8)	0.0208 (8)	0.0237 (8)	-0.0008 (6)	0.0044 (6)	0.0015 (6)
0.0179 (8)	0.0212 (8)	0.0252 (8)	-0.0014 (6)	0.0064 (6)	0.0007 (6)
0.0193 (8)	0.0214 (8)	0.0298 (9)	-0.0019 (6)	0.0089 (7)	-0.0019 (7)
0.0184 (8)	0.0210 (8)	0.0257 (8)	-0.0005 (6)	0.0048 (6)	0.0010 (6)
0.0450 (10)	0.0423 (10)	0.0376 (9)	-0.0045 (8)	0.0090 (8)	0.0027 (7)
0.0369 (9)	0.0359 (8)	0.0366 (9)	-0.0010 (7)	0.0110 (7)	-0.0037 (7)
0.0394 (9)	0.0319 (8)	0.0336 (8)	-0.0028 (7)	0.0090 (7)	0.0072 (6)
0.0375 (9)	0.0368 (8)	0.0325 (8)	-0.0023 (7)	0.0077 (7)	0.0000 (7)
0.0410 (9)	0.0326 (8)	0.0431 (9)	0.0008 (7)	0.0208 (7)	-0.0011 (7)
0.0474 (10)	0.0411 (9)	0.0446 (10)	-0.0062 (8)	0.0126 (8)	0.0076 (8)
0.0298 (8)	0.0358 (8)	0.0285 (8)	-0.0037 (6)	0.0042 (6)	-0.0007 (6)
0.0182 (9)	0.0256 (9)	0.0189 (9)	-0.0012 (7)	0.0040 (7)	-0.0002 (7)
0.0192 (10)	0.0261 (10)	0.0352 (11)	0.0016 (8)	0.0064 (8)	-0.0005 (8)
0.0211 (10)	0.0243 (10)	0.0342 (11)	0.0051 (8)	0.0050 (8)	0.0009 (8)
0.0201 (9)	0.0217 (9)	0.0217 (9)	0.0019 (7)	0.0040 (7)	0.0017 (7)
0.0214 (9)	0.0224 (9)	0.0203 (9)	0.0005 (7)	0.0037 (7)	0.0011 (7)
0.0223 (9)	0.0223 (9)	0.0190 (9)	-0.0008 (7)	0.0056 (7)	0.0003 (7)
0.0254 (10)	0.0210 (9)	0.0280 (10)	-0.0030 (8)	0.0076 (8)	0.0011 (8)
0.0225 (10)	0.0254 (10)	0.0284 (10)	-0.0053 (8)	0.0103 (8)	0.0010 (8)
	U^{11} 0.01691 (8) 0.0182 (8) 0.0179 (8) 0.0193 (8) 0.0184 (8) 0.0450 (10) 0.0369 (9) 0.0375 (9) 0.0410 (9) 0.0474 (10) 0.0298 (8) 0.0192 (10) 0.0211 (10) 0.0211 (10) 0.0214 (9) 0.0223 (9) 0.0254 (10) 0.0225 (10)	U^{11} U^{22} $0.01691 (8)$ $0.02131 (8)$ $0.0182 (8)$ $0.0208 (8)$ $0.0179 (8)$ $0.0212 (8)$ $0.0179 (8)$ $0.0212 (8)$ $0.0193 (8)$ $0.0214 (8)$ $0.0184 (8)$ $0.0210 (8)$ $0.0450 (10)$ $0.0423 (10)$ $0.0369 (9)$ $0.0359 (8)$ $0.0375 (9)$ $0.0368 (8)$ $0.0410 (9)$ $0.0326 (8)$ $0.0474 (10)$ $0.0411 (9)$ $0.0298 (8)$ $0.0358 (8)$ $0.0192 (10)$ $0.0261 (10)$ $0.0211 (10)$ $0.0217 (9)$ $0.0214 (9)$ $0.0223 (9)$ $0.0254 (10)$ $0.0254 (10)$	U^{11} U^{22} U^{33} 0.01691 (8)0.02131 (8)0.02469 (8)0.0182 (8)0.0208 (8)0.0237 (8)0.0179 (8)0.0212 (8)0.0252 (8)0.0193 (8)0.0214 (8)0.0298 (9)0.0184 (8)0.0210 (8)0.0257 (8)0.0450 (10)0.0423 (10)0.0376 (9)0.0369 (9)0.0359 (8)0.0366 (9)0.0375 (9)0.0368 (8)0.0325 (8)0.0410 (9)0.0326 (8)0.0431 (9)0.0474 (10)0.0411 (9)0.0446 (10)0.0298 (8)0.0256 (9)0.0189 (9)0.0192 (10)0.0261 (10)0.0352 (11)0.0211 (10)0.0243 (10)0.0342 (11)0.0214 (9)0.0224 (9)0.0203 (9)0.0223 (9)0.0223 (9)0.0190 (9)0.0254 (10)0.0254 (10)0.0284 (10)	U^{11} U^{22} U^{33} U^{12} 0.01691 (8)0.02131 (8)0.02469 (8) -0.00051 (5)0.0182 (8)0.0208 (8)0.0237 (8) -0.0008 (6)0.0179 (8)0.0212 (8)0.0252 (8) -0.0014 (6)0.0193 (8)0.0214 (8)0.0298 (9) -0.0019 (6)0.0184 (8)0.0210 (8)0.0257 (8) -0.0005 (6)0.0450 (10)0.0423 (10)0.0376 (9) -0.0045 (8)0.0369 (9)0.0359 (8)0.0366 (9) -0.0028 (7)0.0375 (9)0.0368 (8)0.0325 (8) -0.0023 (7)0.0410 (9)0.0326 (8)0.0431 (9) 0.0008 (7)0.0474 (10)0.0411 (9) 0.0446 (10) -0.0062 (8)0.0298 (8)0.0256 (9) 0.0189 (9) -0.0012 (7)0.0192 (10) 0.0261 (10) 0.0342 (11) 0.0016 (8)0.0211 (10) 0.0217 (9) 0.0217 (9) 0.0005 (7) 0.0223 (9) 0.0223 (9) 0.0233 (9) -0.0008 (7) 0.0223 (9) 0.0223 (9) 0.0233 (9) -0.0037 (6) 0.0223 (9) 0.0223 (9) 0.0203 (9) -0.0008 (7) 0.0223 (9) 0.0223 (9) 0.0203 (9) -0.0008 (7) 0.0254 (10) 0.0254 (10) -0.0233 (8)	U^{11} U^{22} U^{33} U^{12} U^{13} $0.01691 (8)$ $0.02131 (8)$ $0.02469 (8)$ $-0.00051 (5)$ $0.00575 (5)$ $0.0182 (8)$ $0.0208 (8)$ $0.0237 (8)$ $-0.0008 (6)$ $0.0044 (6)$ $0.0179 (8)$ $0.0212 (8)$ $0.0252 (8)$ $-0.0014 (6)$ $0.0064 (6)$ $0.0193 (8)$ $0.0214 (8)$ $0.0298 (9)$ $-0.0019 (6)$ $0.0089 (7)$ $0.0184 (8)$ $0.0210 (8)$ $0.0257 (8)$ $-0.0005 (6)$ $0.0048 (6)$ $0.0450 (10)$ $0.0423 (10)$ $0.0376 (9)$ $-0.0045 (8)$ $0.0090 (8)$ $0.0369 (9)$ $0.0359 (8)$ $0.0366 (9)$ $-0.0010 (7)$ $0.0110 (7)$ $0.0369 (9)$ $0.0319 (8)$ $0.0336 (8)$ $-0.0023 (7)$ $0.0090 (7)$ $0.0375 (9)$ $0.0368 (8)$ $0.0325 (8)$ $-0.0023 (7)$ $0.0077 (7)$ $0.0410 (9)$ $0.0326 (8)$ $0.0431 (9)$ $0.0008 (7)$ $0.0208 (7)$ $0.0474 (10)$ $0.0411 (9)$ $0.0446 (10)$ $-0.0062 (8)$ $0.0126 (8)$ $0.0298 (8)$ $0.0358 (8)$ $0.0285 (8)$ $-0.0037 (6)$ $0.0040 (7)$ $0.0192 (10)$ $0.0261 (10)$ $0.0322 (11)$ $0.0016 (8)$ $0.0064 (8)$ $0.0201 (9)$ $0.0217 (9)$ $0.0217 (9)$ $0.0019 (7)$ $0.0037 (7)$ $0.0223 (9)$ $0.0223 (9)$ $0.0190 (9)$ $-0.0008 (7)$ $0.0056 (7)$ $0.0223 (9)$ $0.0223 (9)$ $0.0203 (9)$ $0.0005 (7)$ $0.0037 (7)$ $0.0224 (10)$ $0.0228 (10)$ $-0.0030 (8)$ $0.0076 (8)$

supporting information

С9	0.0202 (9)	0.0238 (9)	0.0213 (9)	-0.0018 (7)	0.0068 (7)	0.0004 (7)
C10	0.0206 (9)	0.0258 (10)	0.0214 (9)	-0.0024 (8)	0.0075 (8)	-0.0015 (7)
C11	0.0197 (9)	0.0250 (10)	0.0233 (10)	-0.0019 (8)	0.0069 (8)	-0.0017 (8)
C12	0.0194 (10)	0.0275 (10)	0.0351 (11)	0.0005 (8)	0.0099 (8)	-0.0007 (8)
C13	0.0240 (10)	0.0229 (9)	0.0349 (11)	0.0022 (8)	0.0107 (9)	-0.0014 (8)
C14	0.0204 (9)	0.0218 (9)	0.0254 (10)	-0.0002(7)	0.0065 (8)	-0.0006 (7)
C15	0.0217 (9)	0.0223 (9)	0.0233 (10)	0.0013 (7)	0.0058 (8)	0.0005 (7)
C16	0.0201 (9)	0.0221 (9)	0.0238 (10)	-0.0009(7)	0.0038 (8)	0.0021 (7)
C17	0.0249 (10)	0.0213 (9)	0.0360 (11)	-0.0030(8)	0.0073 (9)	0.0028 (8)
C18	0.0196 (10)	0.0256 (10)	0.0345 (11)	-0.0040(8)	0.0074 (8)	0.0020 (8)
C19	0.0187 (9)	0.0247 (10)	0.0219 (9)	-0.0017(7)	0.0032 (7)	0.0019 (7)
C20	0.0172 (9)	0.0249 (9)	0.0191 (9)	-0.0014(7)	0.0025 (7)	0.0014 (7)
C21	0.0170(9)	0.0231(9)	0.0261 (10)	-0.0010(7)	0.0051(7)	-0.0011(8)
C22	0.0223(10)	0.0309(10)	0.0293(11)	-0.0004(8)	0.0051 (8)	0.0035 (8)
C23	0.0228(11)	0.0306(11)	0.0394(12)	-0.0032(9)	0.0139(9)	0.001(0)
C24	0.0180(10)	0.0322(11)	0.0472(13)	-0.0034(8)	0.0097 (9)	-0.0044(10)
C25	0.0195(10)	0.0349(11)	0.0357(12)	0.0010 (9)	0.0014 (9)	-0.0008(9)
C26	0.0207(10)	0.0297(10)	0.0258(10)	0.0010(3)	0.0011(9) 0.0048(8)	0.0009 (8)
C27	0.0166 (9)	0.023(9)	0.0230(10) 0.0275(10)	-0.0002(7)	0.0023 (8)	0.0000 (0) 0.0021 (8)
C28	0.0219(10)	0.0223(9)	0.0215(11)	0.0002(7)	0.0029(8)	0.0021(8)
C29	0.0247(11)	0.0201(10) 0.0272(10)	0.0313(11) 0.0441(13)	0.0012 (8)	0.0039(0)	-0.0029(0)
C30	0.0268(11)	0.02/2(10)	0.0567(15)	0.0032(0)	0.0000(0)	0.0052(10)
C31	0.0200(11) 0.0378(13)	0.0201(10) 0.0307(11)	0.0307(13) 0.0427(13)	0.0021(0) 0.0030(10)	0.0077(10)	0.0032(10) 0.0135(10)
C32	0.0342(12)	0.0309(11)	0.0127(13) 0.0290(11)	0.0030(10)	0.0067 (9)	0.0133(10) 0.0041(9)
C33	0.0312(12)	0.0186 (9)	0.0290(11) 0.0284(10)	-0.0013(7)	0.0089 (8)	0.0011(7)
C34	0.0202(9)	0.0100(9) 0.0272(10)	0.0204(10) 0.0291(11)	-0.0013(7)	0.0109 (8)	-0.0040(8)
C35	0.0237(10)	0.0272(10) 0.0270(10)	0.0291(11) 0.0368(12)	-0.0027(8)	0.0105(0)	-0.0053(9)
C36	0.0232(10) 0.0217(10)	0.0270(10) 0.0221(10)	0.0300(12) 0.0473(13)	-0.0016(8)	0.0010(9)	0.0007(9)
C37	0.0322(12)	0.0450(13)	0.0370(12)	-0.0047(10)	0.0206(10)	-0.0057(10)
C38	0.0322(12) 0.0270(11)	0.0458(13)	0.0270(12) 0.0281(11)	-0.0070(10)	0.0096 (9)	-0.0088(10)
C39	0.0184(9)	0.0210(9)	0.0306(10)	-0.0020(7)	0.0102 (8)	0 0004 (8)
C40	0.0268(11)	0.0250(10)	0.0317(11)	-0.0002(8)	0.0024(9)	-0.0031(8)
C41	0.0263(11)	0.0257(10)	0.0428(13)	0.0032 (8)	0.0021(9)	0.0055 (9)
C42	0.0296(11)	0.0227(10) 0.0214(10)	0.0504(14)	-0.0008(8)	0.0010(0)	-0.0024(9)
C43	0.0529(15)	0.0298(11)	0.0347(12)	-0.0065(10)	0.0154(11)	-0.0078(9)
C44	0.0456(13)	0.0292(11)	0.0282(11)	-0.0024(10)	0.0083(10)	0.0034 (9)
C45	0.0467(14)	0.0291(11)	0.0405(13)	0.0064 (10)	0.0131(11)	-0.0001(10)
C46	0.0492(14)	0.0264(11)	0.0397(13)	0.0029 (10)	0.0116(11)	0.0038 (9)
C47	0.0470(14)	0.0343(12)	0.0437(14)	-0.0072(11)	0.0161(11)	0.0073(10)
C48	0.0406 (13)	0.0373(13)	0.0425(13)	-0.0105(10)	0.0113(11)	0.0016(10)
C49	0.0294(12)	0.0275(14)	0.0398(13)	0 0004 (10)	0.0136(10)	0.0032(10)
C50	0.0291(12) 0.0400(14)	0.0463(14)	0.0510(15)	0.0061 (11)	0.0252(12)	0.0022(10)
C51	0.0558 (16)	0.0314(12)	0.0638(17)	0.0038(11)	0.0256(14)	-0.0040(12)
C52	0.0582(17)	0.0318(12)	0.0572 (16)	0.0004 (12)	0.0207 (13)	0.0022 (11)
C53	0.0519(15)	0.0332(12)	0.0506(15)	-0.0068(11)	0.0163(12)	0.0047(11)
C54	0.0416(14)	0.0375(12)	0.0428(14)	-0.0119(11)	0.0073(11)	-0.0024(10)
C55	0.0256(11)	0.0472(14)	0.0342(12)	-0.0020(10)	-0.0001(9)	0.0015(10)
C56	0.0250(11)	0.0465(13)	0.0012(12) 0.0406(13)	0.0020(10)	0.0001(9)	0.0010(10)
000	0.0201 (11)	0.0102 (12)	0.0100(15)	0.0070(10)	0.0000 (10)	0.0021 (10)

Geometric parameters (Å, °)

$\begin{array}{cccccccccccccccccccccccccccccccccccc$					
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Cd—N1	2.2296 (15)	C25—C26	1.387 (3)	
Cd-N32.2322 (16)C26-H260.9500Cd-N42.2265 (15)C27-C281.395 (3)Cd-O12.2368 (18)C27-C221.399 (3)N1-C41.367 (2)C28-C291.388 (3)N1-C11.370 (2)C28-H280.9500N2-C61.369 (2)C29-C301.385 (3)N2-C791.370 (2)C29-H290.9500N3-C141.366 (2)C30-C311.381 (3)N3-C141.366 (2)C31-C321.386 (3)N4-C161.368 (2)C31-C321.386 (3)N4-C191.371 (2)C31-H310.9500O1-H1011.004 (10)C32-H320.9500O1-H1010.996 (10)C33-C341.390 (3)O2-C451.413 (3)C33-C381.393 (3)O2-C451.417 (3)C34-C351.395 (3)O3-C471.424 (3)C35-H350.9500O3-C471.424 (3)C35-H350.9500O3-C471.424 (3)C36-C371.378 (3)O5-C511.407 (3)C36-C371.378 (3)O5-C501.417 (3)C37-C381.384 (3)O5-C511.420 (3)C39-C441.390 (3)O7-C551.422 (3)C39-C441.390 (3)C1-C201.420 (3)C40-C411.388 (3)C1-C21.450 (3)C40-C411.388 (3)C1-C21.450 (3)C40-C411.388 (3)C1-C21.450 (3)C40-C411.388 (3)C2-C41.451 (3)C42-C431.384 (3) <t< td=""><td>Cd—N2</td><td>2.2296 (15)</td><td>C25—H25</td><td>0.9500</td><td></td></t<>	Cd—N2	2.2296 (15)	C25—H25	0.9500	
Cd-N42.2265 (15)C27-C281.395 (3)Cd-O12.2368 (18)C27-C321.398 (3)N1-C41.367 (2)C28-C291.388 (3)N1-C11.370 (2)C28-H280.9500N2-C61.369 (2)C29-C301.385 (3)N2-C91.370 (2)C29-H290.9500N3-C141.366 (2)C30-C311.381 (3)N3-C111.368 (2)C31-C321.386 (3)N4-C161.368 (2)C31-C320.9500N4-C191.371 (2)C31-H310.9500O1-H1011.004 (10)C32-H320.9500O2-C451.413 (3)C33-C341.393 (3)O2-C451.413 (3)C33-C341.395 (3)O2-C451.413 (3)C34-C351.395 (3)O2-C461.416 (3)C34-H340.9500O3-C471.424 (3)C35-C361.375 (3)O4-C481.414 (3)C35-H350.9500O5-C511.407 (3)C37-C381.384 (3)O5-C501.417 (3)C37-C381.384 (3)O6-C521.420 (3)C39-C441.390 (3)O7-C541.420 (3)C39-C441.390 (3)O7-C541.420 (3)C40-C411.388 (3)C1-C201.420 (3)C40-C411.388 (3)C1-C201.420 (3)C40-C411.388 (3)C1-C201.420 (3)C40-C411.388 (3)C1-C201.420 (3)C40-C411.388 (3)C1-C201.423 (3)C40-C411.388 (3) <t< td=""><td>Cd—N3</td><td>2.2322 (16)</td><td>C26—H26</td><td>0.9500</td><td></td></t<>	Cd—N3	2.2322 (16)	C26—H26	0.9500	
Cd-O12.2368 (18)C27-C321.399 (3)N1-C41.367 (2)C28-C291.388 (3)N1-C11.370 (2)C28-H280.9500N2-C61.369 (2)C29-G301.385 (3)N2-C71.370 (2)C29-H290.9500N3-C141.368 (2)C30-H300.9500N4-C161.368 (2)C31-H310.9500O1-H1011.004 (10)C32-H320.9500O1-H1010.096 (10)C33-C341.390 (3)O2-C451.413 (3)C33-C381.393 (3)O2-C451.416 (3)C34-H340.9500O3-C461.416 (3)C34-H340.9500O3-C461.416 (3)C34-H340.9500O4-C491.419 (3)C35-C361.375 (3)O4-C491.419 (3)C36-C371.378 (3)O5-C511.407 (3)C36-H360.9500O4-C491.419 (3)C36-H360.9500O5-C521.409 (3)C37-C181.384 (3)O6-C531.434 (3)C39-C441.390 (3)O7-C541.420 (3)C39-C441.390 (3)C1-C21.450 (3)C40-H400.9500C2-C31.352 (3)C41-C421.378 (3)C2-C41.451 (3)C42-C431.384 (3)C3-C41.451 (3)C42-C431.384 (3)C5-C61.423 (3)C43-H430.9500C5-C61.423 (3)C43-H440.9500C5-C61.423 (3)C45-C461.502 (3)C5-C61.447 (3	Cd—N4	2.2265 (15)	C27—C28	1.395 (3)	
N1C4 $1.367 (2)$ $C28C29$ $1.388 (3)$ N1C1 $1.370 (2)$ $C28H28$ 0.9500 N2C6 $1.369 (2)$ $C29C30$ $1.385 (3)$ N2C9 $1.370 (2)$ $C29-H29$ 0.9500 N3C14 $1.366 (2)$ $C30C31$ $1.381 (3)$ N3C16 $1.368 (2)$ $C30-H30$ 0.9500 N4C16 $1.368 (2)$ $C31C32$ $1.386 (3)$ N4C16 $1.368 (2)$ $C31C32$ $1.386 (3)$ O1-H101 $1.004 (10)$ $C32-H32$ 0.9500 O1-H201 $0.996 (10)$ $C33C34$ $1.390 (3)$ O2C45 $1.413 (3)$ $C33C38$ $1.393 (3)$ O2C45 $1.413 (3)$ $C34C35$ $1.395 (3)$ O2C46 $1.416 (3)$ $C34-H34$ 0.9500 O3C47 $1.424 (3)$ $C35-C36$ $1.375 (3)$ O4-C48 $1.414 (3)$ $C35-H35$ 0.9500 O4-C48 $1.419 (3)$ $C36-H36$ 0.9500 O4-C48 $1.419 (3)$ $C36-H36$ 0.9500 O5-C50 $1.417 (3)$ $C37-H37$ 0.9500 O5-C50 $1.417 (3)$ $C39-C44$ $1.390 (3)$ O7-C54 $1.420 (3)$ $C39-C44$ $1.390 (3)$ O7-C55 $1.422 (3)$ $C39-C44$ $1.387 (3)$ C2-C42 $1.352 (3)$ C41-C42 $1.378 (3)$ C2-C5 $1.417 (3)$ C42-C43 $1.384 (3)$ C3-C4 $1.451 (3)$ C42-C43 $1.384 (3)$ C3-C5 $1.422 (3)$ C40-C41 $1.387 (3)$	Cd—01	2.2368 (18)	C27—C32	1.399 (3)	
N1C1 1.370 (2) $C28-H28$ 0.9500 N2C6 1.369 (2) $C29-C30$ 1.385 (3)N2C7 1.370 (2) $C29-H29$ 0.9500 N3C14 1.366 (2) $C30-C31$ 1.381 (3)N3C11 1.366 (2) $C31-C32$ 1.386 (3)N4C16 1.368 (2) $C31-H31$ 0.9500 O1-H101 1.004 (10) $C32-H32$ 0.9500 O1-H201 0.996 (10) $C33-C34$ 1.390 (3)O2C45 1.413 (3) $C33-C38$ 1.393 (3)O2C56 1.417 (3) $C34-C35$ 1.395 (3)O3-C47 1.424 (3) $C35-H35$ 0.9500 O4C48 1.414 (3) $C35-H35$ 0.9500 O4-C48 1.414 (3) $C35-H35$ 0.9500 O4-C49 1.419 (3) $C36-C37$ 1.378 (3)O5-C51 1.407 (3) $C36-H36$ 0.9500 O5-C52 1.409 (3) $C37-H37$ 0.9500 O6-C53 1.434 (3) $C38-H38$ 0.9500 O7-C55 1.422 (3) $C39-C44$ 1.390 (3)C1-C20 1.420 (3) $C40-C41$ 1.388 (3)C1-C2 1.450 (3) $C40-C41$ 1.388 (3)C2-C5 1.417 (3) $C42-C43$ 1.384 (3)C3-C4 1.451 (3) $C42-C43$ 1.384 (3)C3-C4 1.451 (3) $C42-C43$ 1.387 (3)C4-C2 1.356 (3) $C40-H44$ 0.9500 C2-C3 1.352 (3) $C40-C41$ 1.387 (3)C2-C43 </td <td>N1—C4</td> <td>1.367 (2)</td> <td>C28—C29</td> <td>1.388 (3)</td> <td></td>	N1—C4	1.367 (2)	C28—C29	1.388 (3)	
N2-C6 $1.369 (2)$ C29-C30 $1.385 (3)$ N2-C9 $1.370 (2)$ C29-H29 0.9500 N3-C14 $1.366 (2)$ C30-C31 $1.381 (3)$ N3-C11 $1.368 (2)$ C31-C32 $1.386 (3)$ N4-C16 $1.368 (2)$ C31-C32 0.9500 O1-H101 $1.004 (10)$ C32-H32 0.9500 O1-H201 $0.996 (10)$ C33-C34 $1.390 (3)$ O2-C45 $1.413 (3)$ C33-C38 $1.393 (3)$ O2-C46 $1.416 (3)$ C34-H34 0.9500 O3-C46 $1.416 (3)$ C34-H34 0.9500 O3-C47 $1.424 (3)$ C35-C36 $1.375 (3)$ O4-C48 $1.414 (3)$ C35-H35 0.9500 O5-C51 $1.407 (3)$ C36-H36 0.9500 O5-C51 $1.407 (3)$ C36-H36 0.9500 O5-C51 $1.407 (3)$ C37-C38 $1.384 (3)$ O5-C51 $1.409 (3)$ C39-C40 $1.390 (3)$ O7-C54 $1.420 (3)$ C39-C40 $1.390 (3)$ O7-C55 $1.422 (3)$ C39-C40 $1.390 (3)$ C1-C2 $1.450 (3)$ C40-C41 $1.388 (3)$ C2-H2 0.9500 C41-C42 $1.378 (3)$ C2-H2 0.9500 C41-C42 $1.378 (3)$ C2-H2 0.9500 C41-C44 $1.387 (3)$ C2-H2 0.9500 C41-C42 $1.378 (3)$ C2-H2 0.9500 C41-C42 0.9500 C3-C4 $1.417 (3)$ C43-C44 $1.387 (3)$ C2-H2 0.9500 C41-C42 0.9500 C3-	N1	1.370 (2)	C28—H28	0.9500	
N2-C9 $1.370 (2)$ $C29-H29$ 0.9500 N3-C14 $1.366 (2)$ $C30-C31$ $1.381 (3)$ N3-C11 $1.368 (2)$ $C30-C31$ $1.381 (3)$ N4-C16 $1.368 (2)$ $C31-C32$ $1.386 (3)$ N4-C19 $1.371 (2)$ $C31-H31$ 0.9500 O1-H101 $1.004 (10)$ $C32-H32$ 0.9500 O1-H201 $0.996 (10)$ $C33-C34$ $1.390 (3)$ O2-C45 $1.413 (3)$ $C33-C38$ $1.395 (3)$ O2-C45 $1.417 (3)$ $C34-C35$ $1.395 (3)$ O3-C46 $1.416 (3)$ $C35-C36$ $1.375 (3)$ O3-C47 $1.424 (3)$ $C35-C36$ $1.375 (3)$ O4-C48 $1.414 (3)$ $C35-H35$ 0.9500 O3-C51 $1.407 (3)$ $C37-C38$ $1.384 (3)$ O5-C50 $1.417 (3)$ $C37-C38$ $1.384 (3)$ O6-C52 $1.409 (3)$ $C37-C38$ $1.384 (3)$ O6-C52 $1.409 (3)$ $C39-C44$ $1.390 (3)$ O7-C54 $1.420 (3)$ $C39-C44$ $1.390 (3)$ O7-C55 $1.422 (3)$ $C39-C44$ $1.390 (3)$ C1-C2 $1.450 (3)$ $C40-C41$ $1.388 (3)$ C2-H2 0.9500 $C41-H41$ 0.9500 C3-C4 $1.451 (3)$ $C42-C43$ $1.384 (3)$ C2-H2 0.9500 $C41-H44$ 0.9500 C3-C4 $1.477 (3)$ $C43-C44$ $1.387 (3)$ C2-H2 0.9500 $C41-H44$ 0.9500 C3-C6 $1.423 (3)$ $C43-C44$ $1.387 (3)$ C3-C6 <td< td=""><td>N2—C6</td><td>1.369 (2)</td><td>C29—C30</td><td>1.385 (3)</td><td></td></td<>	N2—C6	1.369 (2)	C29—C30	1.385 (3)	
N3-C141.366 (2)C30-C311.381 (3)N3-C111.368 (2)C30-H300.9500N4-C161.368 (2)C31-C321.386 (3)N4-C191.371 (2)C31-H310.9500O1-H1011.004 (10)C32-H320.9500O1-H2010.996 (10)C33-C341.390 (3)O2-C451.413 (3)C34-C351.395 (3)O3-C461.416 (3)C34-C351.395 (3)O3-C471.424 (3)C35-C361.375 (3)O4-C481.414 (3)C35-C361.375 (3)O4-C491.419 (3)C36-C371.378 (3)O5-C511.407 (3)C36-H360.9500O5-C501.417 (3)C37-C381.384 (3)O6-C521.409 (3)C39-C441.390 (3)O7-C541.420 (3)C39-C401.390 (3)O7-C551.422 (3)C39-C401.390 (3)C1-C201.420 (3)C40-C411.388 (3)C2-C31.352 (3)C41-C421.378 (3)C2-C41.451 (3)C42-C431.384 (3)C3-C41.451 (3)C42-C461.502 (3) <tr< td=""><td>N2—C9</td><td>1.370 (2)</td><td>C29—H29</td><td>0.9500</td><td></td></tr<>	N2—C9	1.370 (2)	C29—H29	0.9500	
N3C111.368 (2)C30-H300.9500N4C161.368 (2)C31C321.386 (3)N4C191.371 (2)C31-H310.9500O1H1011.004 (10)C32-H320.9500O1H2010.996 (10)C33C341.390 (3)O2C451.413 (3)C33C381.393 (3)O2C451.417 (3)C34C351.395 (3)O3C461.416 (3)C34H340.9500O3C471.424 (3)C35C361.375 (3)O4C481.419 (3)C35H350.9500O4C491.419 (3)C36C371.378 (3)O5C511.407 (3)C37C381.384 (3)O5-C501.417 (3)C37C381.384 (3)O6C521.409 (3)C37H370.9500O7C541.422 (3)C39C441.390 (3)C1C201.420 (3)C40C411.388 (3)C1C21.450 (3)C40C411.388 (3)C2H20.9500C41C421.378 (3)C2H20.9500C41C421.378 (3)C2H20.9500C41C431.384 (3)C3H30.9500C42H431.384 (3)C3H30.9500C42H440.9500C4C51.417 (3)C43C441.387 (3)C5C61.423 (3)C43C441.387 (3)C5C61.423 (3)C43H45A0.9900C5C71.447 (3)C45H45A0.9900C5C71.447 (3)C45H46A	N3—C14	1.366 (2)	C30—C31	1.381 (3)	
N4—C161.368 (2)C31—C321.386 (3)N4—C191.371 (2)C31—H310.9500O1—H1011.004 (10)C32—H320.9500O1—H2010.996 (10)C33—C341.390 (3)O2—C451.413 (3)C33—C381.393 (3)O2—C561.417 (3)C34—C351.395 (3)O3—C461.416 (3)C34—H340.9500O3—C471.424 (3)C35—H350.9500O4—C481.414 (3)C35—H350.9500O4—C481.417 (3)C36—C371.378 (3)O5—C511.407 (3)C36—H360.9500O6—C521.409 (3)C37—H370.9500O6—C531.434 (3)C38—H380.9500O7—C541.420 (3)C39—C441.390 (3)C1—C201.420 (3)C39—C411.388 (3)C1—C21.450 (3)C40—H400.9500C2—C31.352 (3)C41—C421.378 (3)C3—H30.9500C41—H410.9500C4—C51.417 (3)C42—C431.384 (3)C3—H30.9500C41—H440.9500C4—C51.417 (3)C43—C441.387 (3)C5—C61.423 (3)C43—H430.9500C4—C51.417 (3)C45—H45A0.9900C5—C271.497 (3)C45—H45A0.9900C5—C271.497 (3)C45—H45B0.9900C5—C271.447 (3)C45—H45B0.9900C5—C271.447 (3)C45—H45B0.9900C6—C71.447 (3)C	N3—C11	1.368 (2)	C30—H30	0.9500	
N4—C19 1.371 (2) $C31$ —H31 0.9500 O1—H101 1.004 (10) $C32$ —H32 0.9500 O1—H201 0.996 (10) $C33$ —C34 1.390 (3)O2—C45 1.413 (3) $C33$ —C38 1.393 (3)O2—C56 1.417 (3) $C34$ —C35 1.395 (3)O3—C46 1.416 (3) $C34$ —H34 0.9500 O3—C47 1.424 (3) $C35$ —C36 1.375 (3)O4—C48 1.414 (3) $C35$ —H35 0.9500 O4—C49 1.419 (3) $C36$ —C37 1.378 (3)O5—C51 1.407 (3) $C36$ —H36 0.9500 O5—C50 1.417 (3) $C37$ —C38 1.384 (3)O6—C52 1.409 (3) $C37$ —H37 0.9500 O7—C54 1.422 (3) $C39$ —C44 1.390 (3)O7—C55 1.422 (3) $C39$ —C40 1.390 (3)C1—C20 1.420 (3) $C40$ —H40 0.9500 C2—C3 1.352 (3) $C41$ —C42 1.378 (3)C2—H2 0.9500 $C41$ —H41 0.9500 C3—C4 1.451 (3) $C42$ —C43 1.384 (3)C3—H3 0.9500 $C42$ —H42 0.9500 C4—C5 1.417 (3) $C43$ —C44 1.387 (3)C5—C6 1.423 (3) $C43$ —H44 0.9500 C5—C7 1.447 (3) $C45$ —C46 1.502 (3)C5—C6 1.325 (3) $C44$ —H44 0.9500 C5—C7 1.447 (3) $C45$ —C46 1.502 (3)C7—C8 1.356 (3) $C45$ —H45A 0.9900 C5—C9 1.447 (3)<	N4—C16	1.368 (2)	C31—C32	1.386 (3)	
01-H1011.004 (10) $C32-H32$ 0.950001-H2010.996 (10) $C33-C34$ 1.390 (3)02-C451.413 (3) $C33-C38$ 1.393 (3)02-C561.417 (3) $C34-C35$ 1.395 (3)03-C461.416 (3) $C34-H34$ 0.950003-C471.424 (3) $C35-C36$ 1.375 (3)04-C481.414 (3) $C35-H35$ 0.950004-C491.419 (3) $C36-C37$ 1.378 (3)05-C511.407 (3) $C36-H36$ 0.950005-C521.409 (3) $C37-H37$ 0.950006-C531.434 (3) $C38-H38$ 0.950007-C541.420 (3) $C39-C44$ 1.390 (3)07-C551.422 (3) $C39-C44$ 1.390 (3)07-C541.420 (3) $C40-C41$ 1.388 (3)01-C201.420 (3) $C40-C41$ 1.388 (3)02-C431.352 (3) $C41-C42$ 1.378 (3)02-C441.451 (3) $C42-C43$ 1.384 (3)03-C441.451 (3) $C42-C43$ 1.384 (3)03-C441.451 (3) $C42-C43$ 1.387 (3)03-C41.417 (3) $C43-C44$ 1.387 (3)03-C41.447 (3) $C45-H45A$ 0.950003-C471.447 (3) $C45-H45A$ 0.990004-C51.417 (3) $C45-H45A$ 0.990005-C61.423 (3) $C43-H44$ 0.950005-C771.447 (3) $C45-H45A$ 0.9900058-C91.447 (3) $C45-H45A$ 0.9900058-C91.447 (3) <td< td=""><td>N4—C19</td><td>1.371 (2)</td><td>C31—H31</td><td>0.9500</td><td></td></td<>	N4—C19	1.371 (2)	C31—H31	0.9500	
01-H201 $0.996(10)$ $C33-C34$ $1.390(3)$ $02-C45$ $1.413(3)$ $C33-C38$ $1.393(3)$ $02-C56$ $1.417(3)$ $C34-C35$ $1.395(3)$ $03-C46$ $1.416(3)$ $C34-H34$ 0.9500 $03-C47$ $1.424(3)$ $C35-C36$ $1.375(3)$ $04-C48$ $1.414(3)$ $C35-H35$ 0.9500 $04-C49$ $1.419(3)$ $C36-C37$ $1.378(3)$ $05-C51$ $1.407(3)$ $C36-H36$ 0.9500 $05-C52$ $1.409(3)$ $C37-C38$ $1.384(3)$ $06-C52$ $1.409(3)$ $C37-H37$ 0.9500 $06-C53$ $1.434(3)$ $C38-H38$ 0.9500 $07-C54$ $1.420(3)$ $C39-C44$ $1.390(3)$ $07-C55$ $1.422(3)$ $C39-C40$ $1.390(3)$ $C1-C20$ $1.420(3)$ $C40-C41$ $1.388(3)$ $C1-C2$ $1.450(3)$ $C40-C41$ $1.388(3)$ $C2-H2$ 0.9500 $C41-H41$ 0.9500 $C2-C3$ $1.352(3)$ $C41-C42$ $1.378(3)$ $C2-H2$ 0.9500 $C41-H41$ 0.9500 $C3-C4$ $1.451(3)$ $C42-C43$ $1.384(3)$ $C3-C4$ $1.471(3)$ $C43-H43$ 0.9500 $C5-C6$ $1.423(3)$ $C43-H43$ 0.9500 $C5-C7$ $1.497(3)$ $C45-H45B$ 0.9900 $C5-C7$ $1.447(3)$ $C45-H46A$ 0.9900 $C5-C7$ $1.447(3)$ $C45-H45B$ 0.9900 $C5-C7$ $1.447(3)$ $C45-H45B$ 0.9900 $C8-C9$ <t< td=""><td>01—H101</td><td>1.004 (10)</td><td>С32—Н32</td><td>0.9500</td><td></td></t<>	01—H101	1.004 (10)	С32—Н32	0.9500	
02-C45 1.413 (a) $C33-C38$ 1.393 (b) $02-C56$ 1.417 (b) $C34-C35$ 1.395 (b) $03-C46$ 1.416 (b) $C34-H34$ 0.9500 $03-C47$ 1.424 (b) $C35-C36$ 1.375 (b) $04-C48$ 1.414 (b) $C35-H35$ 0.9500 $04-C49$ 1.419 (b) $C36-C37$ 1.378 (b) $05-C51$ 1.407 (c) $C36-H36$ 0.9500 $05-C50$ 1.417 (c) $C37-C38$ 1.384 (c) $06-C52$ 1.409 (c) $C37-H37$ 0.9500 $06-C53$ 1.422 (c) $C39-C44$ 1.390 (c) $07-C54$ 1.420 (c) $C39-C40$ 1.390 (c) $07-C55$ 1.422 (c) $C39-C40$ 1.390 (c) $07-C55$ 1.422 (c) $C40-C41$ 1.388 (c) $07-C55$ 1.422 (c) 0.9500 $C41-H41$ 0.9500 $C41-H41$ 0.9500 $C2-C3$ 1.352 (c) $C43-C43$ 1.384 (c) $C3-C4$ 1.451 (c) $C43-C44$ 1.387 (c) $C3-C4$ 1.451 (c) $C43-C44$ 0.9500 $C4-C5$ 1.417 (c) $C43-C44$ 0.9500 $C5-C6$ 1.423 (c) $C43-C44$ 0.9500 $C5-C7$ 1.447 (c) $C45-C46$ 1.502 (c)	01—H2O1	0.996 (10)	C33—C34	1.390 (3)	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O2—C45	1.413 (3)	C33—C38	1.393 (3)	
03C461.416 (3)C34H340.950003C471.424 (3)C35C361.375 (3)04C481.414 (3)C35H350.950004C491.419 (3)C36C371.378 (3)05C511.407 (3)C36H360.950005C501.417 (3)C37C381.384 (3)06C521.409 (3)C37H370.950006C531.434 (3)C38H380.950007C541.420 (3)C39C441.390 (3)07C551.422 (3)C39C401.390 (3)07C551.420 (3)C40C411.388 (3)C1C21.450 (3)C40C411.388 (3)C2C31.352 (3)C41C421.378 (3)C2-H20.9500C41H410.9500C3C41.451 (3)C42C431.384 (3)C3-H30.9500C42H420.9500C4C51.417 (3)C43C441.387 (3)C5-C61.423 (3)C43H430.9500C4C71.447 (3)C45C461.502 (3)C7C81.356 (3)C45H45A0.9900C7C71.447 (3)C45H45B0.9900C7C81.356 (3)C45H45B0.9900C8C91.447 (3)C46H46B0.9900C8C91.447 (3)C46H46B0.9900C8C101.411 (3)C47C481.498 (3)	O2—C56	1.417 (3)	C34—C35	1.395 (3)	
03C471.424 (3)C35C361.375 (3)04C481.414 (3)C35H350.950004C491.419 (3)C36C371.378 (3)05C511.407 (3)C36H360.950005C501.417 (3)C37C381.384 (3)06C521.409 (3)C37H370.950006C531.434 (3)C38H380.950007C541.420 (3)C39C441.390 (3)07C551.422 (3)C39C401.390 (3)07C551.422 (3)C40C411.388 (3)C1C201.420 (3)C40C411.388 (3)C2C31.352 (3)C41C421.378 (3)C2C41.451 (3)C42C431.384 (3)C3C41.451 (3)C42C431.384 (3)C3C51.417 (3)C43C441.387 (3)C3C61.423 (3)C43H430.9500C4C51.417 (3)C43H440.9500C5C271.497 (3)C44H440.9500C6C71.447 (3)C45C461.502 (3)C7C81.356 (3)C45H45A0.9900C7H70.9500C45H45B0.9900C8C91.447 (3)C46H46A0.9900C8C91.447 (3)C46H46B0.9900C8C101.411 (3)C47C481.498 (3)	O3—C46	1.416 (3)	C34—H34	0.9500	
04C48 1.414 (3) $C35-H35$ 0.9500 $04C49$ 1.419 (3) $C36-C37$ 1.378 (3) $05-C51$ 1.407 (3) $C36-H36$ 0.9500 $05-C50$ 1.417 (3) $C37-C38$ 1.384 (3) $06-C52$ 1.409 (3) $C37-H37$ 0.9500 $06-C53$ 1.434 (3) $C38-H38$ 0.9500 $07-C54$ 1.420 (3) $C39-C44$ 1.390 (3) $07-C55$ 1.422 (3) $C39-C44$ 1.390 (3) $C1-C20$ 1.420 (3) $C40-H40$ 0.9500 $C2-C3$ 1.352 (3) $C41-C42$ 1.378 (3) $C2-H2$ 0.9500 $C41-H41$ 0.9500 $C3-C4$ 1.451 (3) $C42-C43$ 1.384 (3) $C3-H3$ 0.9500 $C42-H42$ 0.9500 $C4-C5$ 1.417 (3) $C43-C44$ 1.387 (3) $C5-C6$ 1.423 (3) $C43-H43$ 0.9500 $C4-C5$ 1.417 (3) $C45-H45A$ 0.9900 $C7-C8$ 1.356 (3) $C45-H45A$ 0.9900 $C7-H7$ 0.9500 $C45-H45B$ 0.9900 $C7-H7$ 0.9500 $C45-H45B$ 0.9900 $C7-H7$ 0.9500 $C45-H45B$ 0.9900 $C7-H7$ 0.9500 $C46-H46A$ 0.9900 $C8-C9$ 1.447 (3) $C46-H46B$ 0.9900 $C8-C9$ 1.447 (3) $C46-H46B$ 0.9900 $C8-C9$ 1.441 (3) $C47-C48$ 1.498 (3)	O3—C47	1.424 (3)	C35—C36	1.375 (3)	
04-C49 1.419 (a) $C36-C37$ 1.378 (b) $05-C51$ 1.407 (b) $C36-H36$ 0.9500 $05-C50$ 1.417 (b) $C37-C38$ 1.384 (b) $06-C52$ 1.409 (c) $C37-H37$ 0.9500 $06-C53$ 1.434 (c) $C38-H38$ 0.9500 $07-C54$ 1.420 (c) $C39-C44$ 1.390 (c) $07-C55$ 1.422 (c) $C39-C40$ 1.390 (c) $07-C55$ 1.422 (c) $C40-C41$ 1.388 (c) $07-C55$ 1.420 (c) $C40-C41$ 1.388 (c) $07-C52$ 1.450 (c) $C40-C41$ 1.388 (c) $07-C53$ 1.352 (c) $C41-C42$ 1.378 (c) $07-C2$ 1.450 (c) $C41-C42$ 1.378 (c) $07-C2$ 1.450 (c) $C42-C43$ 1.384 (c) $07-C2$ 1.451 (c) $C42-C43$ 1.384 (c) $07-C2$ 1.417 (c) $C43-C44$ 1.387 (c) $07-C5$ 1.417 (c) $C43-C44$ 1.387 (c) $07-C5$ 1.447 (c) $C43-C44$ 1.387 (c) $07-C6$ 1.423 (c) $C45-C46$ 1.502 (c) $07-C8$ 1.356 (c) $C45-C46$ 1.502 (c) $07-C8$ 1.356 (c) $C45-H45A$ 0.9900 $07-C8$ 1.447 (c) $C46-H46A$ 0.9900 $08-C9$ 1.447 (c)	O4—C48	1.414 (3)	С35—Н35	0.9500	
05-C51 $1.407 (3)$ $C36-H36$ 0.9500 $05-C50$ $1.417 (3)$ $C37-C38$ $1.384 (3)$ $06-C52$ $1.409 (3)$ $C37-H37$ 0.9500 $06-C53$ $1.434 (3)$ $C38-H38$ 0.9500 $07-C54$ $1.420 (3)$ $C39-C44$ $1.390 (3)$ $07-C55$ $1.422 (3)$ $C39-C40$ $1.390 (3)$ $C1-C20$ $1.420 (3)$ $C40-C41$ $1.388 (3)$ $C1-C2$ $1.450 (3)$ $C40-H40$ 0.9500 $C2-C3$ $1.352 (3)$ $C41-C42$ $1.378 (3)$ $C2-H2$ 0.9500 $C41-H41$ 0.9500 $C3-C4$ $1.451 (3)$ $C42-C43$ $1.384 (3)$ $C3-H3$ 0.9500 $C42-H42$ 0.9500 $C4-C5$ $1.417 (3)$ $C43-C44$ $1.387 (3)$ $C5-C6$ $1.423 (3)$ $C43-H43$ 0.9500 $C5-C77$ $1.447 (3)$ $C45-C46$ $1.502 (3)$ $C7-C8$ $1.356 (3)$ $C45-H45A$ 0.9900 $C7-H7$ 0.9500 $C45-H45B$ 0.9900 $C7-H7$ 0.9500 $C45-H45B$ 0.9900 $C8-C9$ $1.447 (3)$ $C46-H46A$ 0.9900 $C8-H8$ 0.9500 $C46-H46B$ 0.9900 $C9-C10$ $1.411 (3)$ $C47-C48$ $1.498 (3)$	O4—C49	1.419 (3)	C36—C37	1.378 (3)	
05-C50 1.417 (3) $C37-C38$ 1.384 (3) $06-C52$ 1.409 (3) $C37-H37$ 0.9500 $06-C53$ 1.434 (3) $C38-H38$ 0.9500 $07-C54$ 1.420 (3) $C39-C44$ 1.390 (3) $07-C55$ 1.422 (3) $C39-C40$ 1.390 (3) $C1-C20$ 1.420 (3) $C40-C41$ 1.388 (3) $C1-C2$ 1.450 (3) $C40-H40$ 0.9500 $C2-C3$ 1.352 (3) $C41-C42$ 1.378 (3) $C2-H2$ 0.9500 $C41-H41$ 0.9500 $C3-C4$ 1.451 (3) $C42-C43$ 1.384 (3) $C3-H3$ 0.9500 $C42-H42$ 0.9500 $C4-C5$ 1.417 (3) $C43-C44$ 1.387 (3) $C5-C6$ 1.423 (3) $C43-H43$ 0.9500 $C5-C7$ 1.447 (3) $C45-C46$ 1.502 (3) $C7-C8$ 1.356 (3) $C45-H45A$ 0.9900 $C7-H7$ 0.9500 $C45-H45B$ 0.9900 $C7-H7$ 0.9500 $C46-H46A$ 0.9900 $C8-C9$ 1.447 (3) $C46-H46B$ 0.9900 $C8-H8$ 0.9500 $C46-H46B$ 0.9900 $C9-C10$ 1.411 (3) $C47-C48$ 1.498 (3)	O5—C51	1.407 (3)	С36—Н36	0.9500	
06-C52 $1.409 (3)$ $C37-H37$ 0.9500 $06-C53$ $1.434 (3)$ $C38-H38$ 0.9500 $07-C54$ $1.420 (3)$ $C39-C44$ $1.390 (3)$ $07-C55$ $1.422 (3)$ $C39-C40$ $1.390 (3)$ $C1-C20$ $1.420 (3)$ $C40-C41$ $1.388 (3)$ $C1-C2$ $1.450 (3)$ $C40-H40$ 0.9500 $C2-C3$ $1.352 (3)$ $C41-C42$ $1.378 (3)$ $C2-H2$ 0.9500 $C41-H41$ 0.9500 $C3-C4$ $1.451 (3)$ $C42-C43$ $1.384 (3)$ $C3-H3$ 0.9500 $C42-H42$ 0.9500 $C4-C5$ $1.417 (3)$ $C43-C44$ $1.387 (3)$ $C5-C6$ $1.423 (3)$ $C43-H43$ 0.9500 $C5-C7$ $1.447 (3)$ $C45-C46$ $1.502 (3)$ $C7-C8$ $1.356 (3)$ $C45-H45A$ 0.9900 $C7-H7$ 0.9500 $C45-H45B$ 0.9900 $C8-C9$ $1.447 (3)$ $C46-H46A$ 0.9900 $C8-H8$ 0.9500 $C46-H46B$ 0.9900 $C9-C10$ $1.411 (3)$ $C47-C48$ $1.498 (3)$	O5—C50	1.417 (3)	C37—C38	1.384 (3)	
06-C53 1.434 (3) $C38-H38$ 0.9500 $07-C54$ 1.420 (3) $C39-C44$ 1.390 (3) $07-C55$ 1.422 (3) $C39-C40$ 1.390 (3) $C1-C20$ 1.420 (3) $C40-C41$ 1.388 (3) $C1-C2$ 1.450 (3) $C40-H40$ 0.9500 $C2-C3$ 1.352 (3) $C41-C42$ 1.378 (3) $C2-H2$ 0.9500 $C41-H41$ 0.9500 $C3-C4$ 1.451 (3) $C42-C43$ 1.384 (3) $C3-H3$ 0.9500 $C42-H42$ 0.9500 $C4-C5$ 1.417 (3) $C43-C44$ 1.387 (3) $C5-C6$ 1.423 (3) $C43-H43$ 0.9500 $C5-C7$ 1.497 (3) $C44-H44$ 0.9500 $C5-C7$ 1.447 (3) $C45-C46$ 1.502 (3) $C7-C8$ 1.356 (3) $C45-H45A$ 0.9900 $C7-H7$ 0.9500 $C45-H45B$ 0.9900 $C8-C9$ 1.447 (3) $C46-H46A$ 0.9900 $C8-H8$ 0.9500 $C46-H46B$ 0.9900 $C9-C10$ 1.411 (3) $C47-C48$ 1.498 (3)	O6—C52	1.409 (3)	С37—Н37	0.9500	
07-C54 1.420 (3) $C39-C44$ 1.390 (3) $07-C55$ 1.422 (3) $C39-C40$ 1.390 (3) $C1-C20$ 1.420 (3) $C40-C41$ 1.388 (3) $C1-C2$ 1.450 (3) $C40-H40$ 0.9500 $C2-C3$ 1.352 (3) $C41-C42$ 1.378 (3) $C2-H2$ 0.9500 $C41-H41$ 0.9500 $C3-C4$ 1.451 (3) $C42-C43$ 1.384 (3) $C3-H3$ 0.9500 $C42-H42$ 0.9500 $C4-C5$ 1.417 (3) $C43-C44$ 1.387 (3) $C5-C6$ 1.423 (3) $C43-H43$ 0.9500 $C5-C27$ 1.497 (3) $C44-H44$ 0.9500 $C5-C27$ 1.497 (3) $C45-C46$ 1.502 (3) $C7-C8$ 1.356 (3) $C45-H45A$ 0.9900 $C7-H7$ 0.9500 $C45-H45B$ 0.9900 $C8-C9$ 1.447 (3) $C46-H46A$ 0.9900 $C8-H8$ 0.9500 $C46-H46B$ 0.9900 $C9-C10$ 1.411 (3) $C47-C48$ 1.498 (3)	O6—C53	1.434 (3)	C38—H38	0.9500	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O7—C54	1.420 (3)	C39—C44	1.390 (3)	
C1C20 $1.420 (3)$ C40C41 $1.388 (3)$ C1C2 $1.450 (3)$ C40H40 0.9500 C2C3 $1.352 (3)$ C41C42 $1.378 (3)$ C2H2 0.9500 C41H41 0.9500 C3C4 $1.451 (3)$ C42C43 $1.384 (3)$ C3H3 0.9500 C42H42 0.9500 C4C5 $1.417 (3)$ C43C44 $1.387 (3)$ C5C6 $1.423 (3)$ C43H43 0.9500 C5C27 $1.497 (3)$ C44H44 0.9500 C6C7 $1.447 (3)$ C45C46 $1.502 (3)$ C7C8 $1.356 (3)$ C45H45B 0.9900 C7H7 0.9500 C45H45B 0.9900 C8C9 $1.447 (3)$ C46H46A 0.9900 C8H8 0.9500 C46H46B 0.9900 C9C10 $1.411 (3)$ C47C48 $1.498 (3)$	07—C55	1.422 (3)	C39—C40	1.390 (3)	
C1-C21.450 (3)C40-H400.9500C2-C31.352 (3)C41-C421.378 (3)C2-H20.9500C41-H410.9500C3-C41.451 (3)C42-C431.384 (3)C3-H30.9500C42-H420.9500C4-C51.417 (3)C43-C441.387 (3)C5-C61.423 (3)C43-H430.9500C5-C71.497 (3)C44-H440.9500C6-C71.447 (3)C45-C461.502 (3)C7-C81.356 (3)C45-H45A0.9900C7-H70.9500C45-H45B0.9900C8-C91.447 (3)C46-H46B0.9900C9-C101.411 (3)C47-C481.498 (3)	C1-C20	1.420 (3)	C40—C41	1.388 (3)	
C2-C3 $1.352(3)$ C41-C42 $1.378(3)$ C2-H2 0.9500 C41-H41 0.9500 C3-C4 $1.451(3)$ C42-C43 $1.384(3)$ C3-H3 0.9500 C42-H42 0.9500 C4-C5 $1.417(3)$ C43-C44 $1.387(3)$ C5-C6 $1.423(3)$ C43-H43 0.9500 C5-C7 $1.497(3)$ C44-H44 0.9500 C6-C7 $1.447(3)$ C45-C46 $1.502(3)$ C7-C8 $1.356(3)$ C45-H45A 0.9900 C7-H7 0.9500 C45-H45B 0.9900 C8-C9 $1.447(3)$ C46-H46A 0.9900 C8-H8 0.9500 C46-H46B 0.9900 C9-C10 $1.411(3)$ C47-C48 $1.498(3)$	C1—C2	1.450 (3)	C40—H40	0.9500	
C2—H20.9500C41—H410.9500C3—C41.451 (3)C42—C431.384 (3)C3—H30.9500C42—H420.9500C4—C51.417 (3)C43—C441.387 (3)C5—C61.423 (3)C43—H430.9500C5—C271.497 (3)C44—H440.9500C6—C71.447 (3)C45—C461.502 (3)C7—C81.356 (3)C45—H45A0.9900C7—H70.9500C45—H45B0.9900C8—C91.447 (3)C46—H46A0.9900C8—H80.9500C46—H46B0.9900C9—C101.411 (3)C47—C481.498 (3)	С2—С3	1.352 (3)	C41—C42	1.378 (3)	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C2—H2	0.9500	C41—H41	0.9500	
C3—H30.9500C42—H420.9500C4—C51.417 (3)C43—C441.387 (3)C5—C61.423 (3)C43—H430.9500C5—C271.497 (3)C44—H440.9500C6—C71.447 (3)C45—C461.502 (3)C7—C81.356 (3)C45—H45A0.9900C7—H70.9500C45—H45B0.9900C8—C91.447 (3)C46—H46A0.9900C8—H80.9500C46—H46B0.9900C9—C101.411 (3)C47—C481.498 (3)	C3—C4	1.451 (3)	C42—C43	1.384 (3)	
C4—C51.417 (3)C43—C441.387 (3)C5—C61.423 (3)C43—H430.9500C5—C271.497 (3)C44—H440.9500C6—C71.447 (3)C45—C461.502 (3)C7—C81.356 (3)C45—H45A0.9900C7—H70.9500C45—H45B0.9900C8—C91.447 (3)C46—H46A0.9900C8—H80.9500C46—H46B0.9900C9—C101.411 (3)C47—C481.498 (3)	С3—Н3	0.9500	C42—H42	0.9500	
C5—C61.423 (3)C43—H430.9500C5—C271.497 (3)C44—H440.9500C6—C71.447 (3)C45—C461.502 (3)C7—C81.356 (3)C45—H45A0.9900C7—H70.9500C45—H45B0.9900C8—C91.447 (3)C46—H46A0.9900C8—H80.9500C46—H46B0.9900C9—C101.411 (3)C47—C481.498 (3)	C4—C5	1.417 (3)	C43—C44	1.387 (3)	
C5—C271.497 (3)C44—H440.9500C6—C71.447 (3)C45—C461.502 (3)C7—C81.356 (3)C45—H45A0.9900C7—H70.9500C45—H45B0.9900C8—C91.447 (3)C46—H46A0.9900C8—H80.9500C46—H46B0.9900C9—C101.411 (3)C47—C481.498 (3)	С5—С6	1.423 (3)	C43—H43	0.9500	
C6—C71.447 (3)C45—C461.502 (3)C7—C81.356 (3)C45—H45A0.9900C7—H70.9500C45—H45B0.9900C8—C91.447 (3)C46—H46A0.9900C8—H80.9500C46—H46B0.9900C9—C101.411 (3)C47—C481.498 (3)	C5—C27	1.497 (3)	C44—H44	0.9500	
C7—C81.356 (3)C45—H45A0.9900C7—H70.9500C45—H45B0.9900C8—C91.447 (3)C46—H46A0.9900C8—H80.9500C46—H46B0.9900C9—C101.411 (3)C47—C481.498 (3)	С6—С7	1.447 (3)	C45—C46	1.502 (3)	
C7—H70.9500C45—H45B0.9900C8—C91.447 (3)C46—H46A0.9900C8—H80.9500C46—H46B0.9900C9—C101.411 (3)C47—C481.498 (3)	С7—С8	1.356 (3)	C45—H45A	0.9900	
C8—C91.447 (3)C46—H46A0.9900C8—H80.9500C46—H46B0.9900C9—C101.411 (3)C47—C481.498 (3)	С7—Н7	0.9500	C45—H45B	0.9900	
C8—H80.9500C46—H46B0.9900C9—C101.411 (3)C47—C481.498 (3)	С8—С9	1.447 (3)	C46—H46A	0.9900	
C9—C10 1.411 (3) C47—C48 1.498 (3)	С8—Н8	0.9500	C46—H46B	0.9900	
	C9—C10	1.411 (3)	C47—C48	1.498 (3)	
C10—C11 1.416 (3) C47—H47A 0.9900	C10—C11	1.416 (3)	C47—H47A	0.9900	
C10—C33 1.500 (3) C47—H47B 0.9900	C10—C33	1.500 (3)	C47—H47B	0.9900	
C11—C12 1.451 (3) C48—H48A 0.9900	C11—C12	1.451 (3)	C48—H48A	0.9900	
C12—C13 1.350 (3) C48—H48B 0.9900	C12—C13	1.350 (3)	C48—H48B	0.9900	

supporting information

C12—H12	0.9500	C49—C50	1.500 (3)
C13—C14	1.452 (3)	C49—H49A	0.9900
C13—H13	0.9500	C49—H49B	0.9900
C14—C15	1.411 (3)	C50—H50A	0.9900
C15—C16	1.417 (3)	C50—H50B	0.9900
C15—C39	1.498 (3)	C51—C52	1.485 (4)
C16—C17	1.449 (3)	C51—H51A	0.9900
C17—C18	1 353 (3)	C51—H51B	0 9900
C17—H17	0.9500	C52—H52A	0.9900
C_{18} C_{19}	1 450 (3)	C52 H52B	0.9900
	0.0500	C52—1152B	1.408(3)
C10_C20	0.9300	C_{52} U_{52}	1.498 (3)
C19 - C20	1.414 (3)	C53—H53A	0.9900
C20-C21	1.499 (2)	С53—Н53В	0.9900
	1.396 (3)	C54—H54A	0.9900
C21—C26	1.396 (3)	C54—H54B	0.9900
C22—C23	1.386 (3)	C55—C56	1.500 (3)
С22—Н22	0.9500	С55—Н55А	0.9900
C23—C24	1.385 (3)	C55—H55B	0.9900
С23—Н23	0.9500	C56—H56A	0.9900
C24—C25	1.383 (3)	C56—H56B	0.9900
C24—H24	0.9500		
N4—Cd—N2	140.94 (6)	C31—C30—C29	119.9 (2)
N4—Cd—N1	83.42 (6)	C31—C30—H30	120.0
N2—Cd—N1	83.30 (6)	C29—C30—H30	120.0
N4—Cd—N3	83.65 (6)	C_{30} $-C_{31}$ $-C_{32}$	120.3 (2)
N2—Cd—N3	83 46 (6)	C_{30} C_{31} H31	119.8
N1—Cd—N3	140 15 (6)	C_{32} C_{31} H31	119.8
NA Cd Ol	11170(6)	C_{32} C_{31} C_{32} C_{27}	119.0 120.0(2)
N_{1} Cd Ol	106.08 (6)	$C_{31} = C_{32} = C_{27}$	120.9 (2)
$N_2 - C_d - O_1$	100.98 (0)	$C_{31} - C_{32} - H_{32}$	119.0
NI-Ca-OI	117.09(0)	$C_2/-C_{32}-H_{32}$	119.0
N3—Cd—Ol	102.71 (6)	$C_{34} - C_{33} - C_{38}$	118.14 (18)
C4—NI—CI	107.92 (15)	C34—C33—C10	121.03 (17)
C4—N1—Cd	124.23 (12)	C38—C33—C10	120.82 (17)
C1—N1—Cd	124.58 (12)	C33—C34—C35	120.72 (19)
C6—N2—C9	107.97 (15)	C33—C34—H34	119.6
C6—N2—Cd	125.45 (12)	C35—C34—H34	119.6
C9—N2—Cd	123.56 (12)	C36—C35—C34	120.10 (19)
C14—N3—C11	108.00 (15)	C36—C35—H35	119.9
C14—N3—Cd	124.12 (12)	С34—С35—Н35	119.9
C11—N3—Cd	123.76 (12)	C35—C36—C37	119.82 (19)
C16—N4—C19	108.22 (15)	С35—С36—Н36	120.1
C16—N4—Cd	124.97 (12)	С37—С36—Н36	120.1
C19—N4—Cd	125.15 (12)	C36—C37—C38	120.2 (2)
Cd-01-H101	112.7 (15)	С36—С37—Н37	119.9
Cd—01—H2O1	112.8 (15)	C38—C37—H37	119.9
H101-01-H201	100(2)	C_{37} — C_{38} — C_{33}	121.0 (2)
C45 - 02 - C56	113 19 (17)	C37_C38_H38	110 5
	112,17 (1/)	0.57 0.50 1150	11/.0

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C46—O3—C47	111.75 (17)	C33—C38—H38	119.5
C48—O4—C49	112.29 (17)	C44—C39—C40	118.30 (18)
C51—O5—C50	112.35 (18)	C44—C39—C15	120.65 (18)
C52—O6—C53	113.09 (18)	C40—C39—C15	121.04 (17)
C54—O7—C55	112.54 (17)	C41—C40—C39	120.65 (19)
N1—C1—C20	125.29 (17)	C41—C40—H40	119.7
N1—C1—C2	108.80 (16)	С39—С40—Н40	119.7
C20—C1—C2	125.88 (17)	C42—C41—C40	120.4 (2)
C3—C2—C1	107.23 (17)	C42—C41—H41	119.8
С3—С2—Н2	126.4	C40—C41—H41	119.8
C1—C2—H2	126.4	C41—C42—C43	119.7 (2)
C2—C3—C4	107.29 (17)	C41—C42—H42	120.1
С2—С3—Н3	126.4	C43—C42—H42	120.1
C4—C3—H3	126.4	C42—C43—C44	119.8 (2)
N1-C4-C5	126 15 (17)	C42—C43—H43	120.1
N1-C4-C3	108 74 (16)	C44 - C43 - H43	120.1
C_{5} C_{4} C_{3}	125.05(17)	C_{43} C_{44} C_{39}	120.1 121.1(2)
C_{3}	125.05(17) 126.64(17)	C_{43} C_{44} H_{44}	121.1(2)
$C_{4} = C_{5} = C_{0}$	116.76 (16)	$C_{43} = C_{44} = H_{44}$	119.4
$C_{4} = C_{5} = C_{27}$	116.70 (10)	$C_{3} = C_{44} = 1144$	117.4
$C_0 - C_3 - C_2 / C_5$	110.00(10) 125.08(17)	02 - C45 - U45 A	109.38 (18)
N2-C6-C3	123.08(17)	02-045-045A	109.8
N2-C0-C7	108.70(10) 126.21(17)	C40 - C45 - H45A	109.8
C_{2}	126.21 (17)	02—C45—H45B	109.8
C8—C/—C6	107.39 (17)	С46—С45—Н45В	109.8
С8—С7—Н7	126.3	H45A—C45—H45B	108.2
С6—С7—Н7	126.3	O3—C46—C45	109.73 (18)
C7—C8—C9	107.17 (17)	O3—C46—H46A	109.7
С7—С8—Н8	126.4	C45—C46—H46A	109.7
С9—С8—Н8	126.4	O3—C46—H46B	109.7
N2—C9—C10	125.80 (17)	C45—C46—H46B	109.7
N2—C9—C8	108.76 (16)	H46A—C46—H46B	108.2
С10—С9—С8	125.40 (17)	O3—C47—C48	109.14 (18)
C9—C10—C11	127.39 (17)	O3—C47—H47A	109.9
C9—C10—C33	116.34 (16)	C48—C47—H47A	109.9
C11—C10—C33	116.22 (16)	O3—C47—H47B	109.9
N3—C11—C10	125.04 (17)	C48—C47—H47B	109.9
N3—C11—C12	108.70 (16)	H47A—C47—H47B	108.3
C10—C11—C12	126.24 (17)	O4—C48—C47	109.48 (19)
C13—C12—C11	107.30 (17)	O4—C48—H48A	109.8
C13—C12—H12	126.4	C47—C48—H48A	109.8
$C_{11} - C_{12} - H_{12}$	126.1	04-C48-H48B	109.8
C12 - C13 - C14	107 26 (17)	C47 - C48 - H48B	109.8
$C_{12} = C_{13} = C_{14}$	107.20 (17)		109.8
$C_{12} - C_{13} - 1113$ $C_{14} - C_{13} - U_{13}$	120.7	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	100.2
$\begin{array}{c} 14 \\ 12 \\ 14 \\ 12 \\ 12 \\ 12 \\ 12 \\ 12 \\$	120.4	04 - 049 - 030	109.2(2)
$1N_{3} - C_{14} - C_{13}$	123.37(17)	04—049—п49А Сбо. С40, 11404	109.8
$1N_{3} - U_{14} - U_{15}$	108./4 (16)	C_{30} C_{49} H_{49} H_{49} H_{49}	109.8
C15—C14—C13	125.67 (17)	04—C49—H49B	109.8
C14-C15-C16	127.11 (17)	C50—C49—H49B	109.8

C14—C15—C39	116.46 (16)	H49A—C49—H49B	108.3
C16—C15—C39	116.39 (16)	O5—C50—C49	108.82 (19)
N4—C16—C15	125.82 (17)	O5—C50—H50A	109.9
N4—C16—C17	108.54 (16)	C49—C50—H50A	109.9
C15—C16—C17	125.62 (18)	O5—C50—H50B	109.9
C18—C17—C16	107.46 (17)	C49—C50—H50B	109.9
C18—C17—H17	126.3	H50A—C50—H50B	108.3
C16—C17—H17	126.3	O5—C51—C52	109.6 (2)
C17—C18—C19	107.28 (17)	O5—C51—H51A	109.7
C17—C18—H18	126.4	С52—С51—Н51А	109.7
C19—C18—H18	126.4	O5—C51—H51B	109.7
N4—C19—C20	125.54 (17)	С52—С51—Н51В	109.7
N4—C19—C18	108.49 (16)	H51A—C51—H51B	108.2
C20-C19-C18	125.86 (17)	O6—C52—C51	109.8 (2)
C19—C20—C1	127.07 (17)	O6—C52—H52A	109.7
C19—C20—C21	116.22 (16)	С51—С52—Н52А	109.7
C1—C20—C21	116.65 (16)	O6—C52—H52B	109.7
C22—C21—C26	118.36 (17)	С51—С52—Н52В	109.7
C22—C21—C20	121.01 (17)	H52A—C52—H52B	108.2
C26—C21—C20	120.62 (17)	O6—C53—C54	109.2 (2)
C23—C22—C21	121.04 (19)	O6—C53—H53A	109.8
C23—C22—H22	119.5	С54—С53—Н53А	109.8
C21—C22—H22	119.5	O6—C53—H53B	109.8
C24—C23—C22	119.9 (2)	С54—С53—Н53В	109.8
С24—С23—Н23	120.1	Н53А—С53—Н53В	108.3
С22—С23—Н23	120.1	O7—C54—C53	109.28 (19)
C25—C24—C23	119.80 (19)	O7—C54—H54A	109.8
C25—C24—H24	120.1	С53—С54—Н54А	109.8
C23—C24—H24	120.1	O7—C54—H54B	109.8
C24—C25—C26	120.5 (2)	C53—C54—H54B	109.8
С24—С25—Н25	119.8	H54A—C54—H54B	108.3
С26—С25—Н25	119.8	O7—C55—C56	109.31 (17)
C25—C26—C21	120.45 (19)	O7—C55—H55A	109.8
С25—С26—Н26	119.8	С56—С55—Н55А	109.8
C21—C26—H26	119.8	O7—C55—H55B	109.8
C28—C27—C32	117.84 (18)	С56—С55—Н55В	109.8
C28—C27—C5	121.36 (17)	Н55А—С55—Н55В	108.3
C32—C27—C5	120.80 (18)	O2—C56—C55	108.82 (19)
C29—C28—C27	121.3 (2)	O2—C56—H56A	109.9
C29—C28—H28	119.3	С55—С56—Н56А	109.9
C27—C28—H28	119.3	O2—C56—H56B	109.9
C30—C29—C28	119.7 (2)	С55—С56—Н56В	109.9
С30—С29—Н29	120.1	H56A—C56—H56B	108.3
С28—С29—Н29	120.1		

Hydrogen-bond geometry (Å, °)

Cg2, Cg3, Cg4 and Cg11 are the centroids of the N2/C6–C9, N3/C11–C14, N4/C16–C19 and C33–C38 rings respectively.

<i>D</i> —H··· <i>A</i>	D—H	H···A	D···A	D—H··· A
01—H1 <i>0</i> 1····O4	1.01 (2)	2.06 (2)	3.057 (2)	176
O1—H2 <i>O</i> 1···O5	1.00 (2)	2.55 (2)	3.138 (2)	118
O1—H2 <i>O</i> 1···O6	1.00 (2)	2.04 (2)	3.013 (2)	165
C31—H31··· <i>Cg</i> 3 ⁱ	0.95	2.93	3.651 (2)	133
C41—H41··· <i>Cg</i> 11 ⁱⁱ	0.95	2.91	3.794 (2)	154
C44—H44··· $Cg2^{iii}$	0.95	2.95	3.648 (2)	131
C47—H47 <i>A</i> ··· <i>Cg</i> 2	0.99	2.91	3.898 (3)	173
C54—H54 <i>B</i> ··· <i>Cg</i> 4	0.99	2.98	3.971 (3)	176

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