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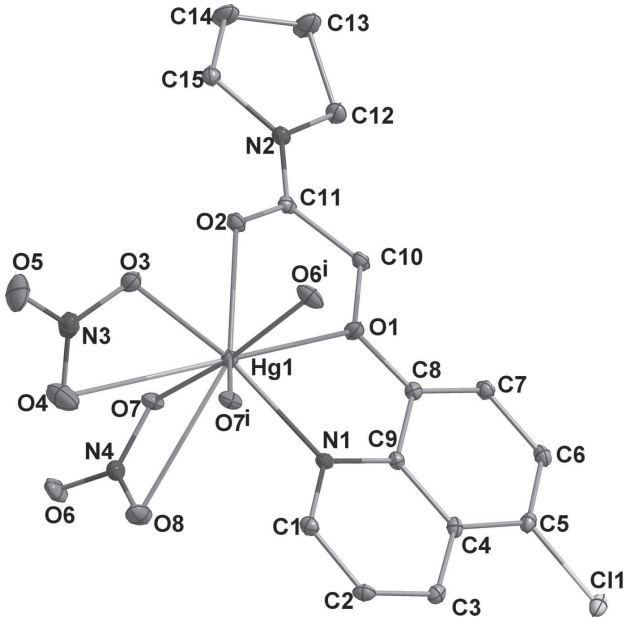
Crystal structure of *catena*-poly[(2-(5-chloroquinolin-8-yloxy)-1-(pyrrolidin-1-yl)ethan-1-one-κ^3*N*,*O*,*O*′)-(dinitrato-κ^2*O*,*O*′)mercury(II)], $C_{15}H_{15}N_4O_8ClHg$



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Abstract

$C_{15}H_{15}N_4O_8ClHg$, monoclinic, $P2_1/n$ (no. 14), $a = 10.660(8)$ Å, $b = 9.523(8)$ Å, $c = 18.275(15)$ Å, $\beta = 99.248(12)°$, $V = 1831(2)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0267$, $wR_{ref}(F^2) = 0.0696$, $T = 296(2)$ K.

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A part of the polymeric title crystal structure is shown in the figure ($^{i} = 0.5 - x$, $0.5 + y$, $1.5 - z$). Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

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Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.10 × 0.08 × 0.06 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	8.61 mm^{-1}
Diffractometer, scan mode:	Bruker SMART, φ and ω-scans
θ_{max}, completeness:	25°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	8815, 3211, 0.031
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2497
$N(param)_{refined}$:	262
Programs:	Bruker [1], SHELX [2]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Hg1	0.32113(2)	0.50498(2)	0.78506(2)	0.03355(9)
Cl1	0.08862(14)	0.60400(15)	1.13121(7)	0.0496(4)
O1	0.3894(3)	0.3909(4)	0.91230(18)	0.0450(9)
O2	0.5047(3)	0.3390(4)	0.80190(19)	0.0401(9)
O3	0.4075(4)	0.5283(4)	0.6841(2)	0.0567(11)
O4	0.2131(6)	0.5380(6)	0.6316(4)	0.102(2)
O5	0.3625(6)	0.5990(6)	0.5718(3)	0.1012(19)
O6	0.0277(4)	0.2265(5)	0.6794(2)	0.0638(12)
O7	0.2015(3)	0.2850(4)	0.75063(19)	0.0431(9)
O8	0.0476(4)	0.4348(5)	0.7274(2)	0.0668(13)
N1	0.2104(3)	0.5810(4)	0.8708(2)	0.0289(9)
N2	0.6257(4)	0.1656(4)	0.8594(2)	0.0360(10)
N3	0.3253(6)	0.5571(6)	0.6275(3)	0.0601(14)
N4	0.0899(4)	0.3176(5)	0.7188(2)	0.0448(11)
C1	0.1213(4)	0.6776(5)	0.8492(3)	0.0358(12)
H1A	0.108113	0.706479	0.799988	0.043*
C2	0.0478(5)	0.7366(5)	0.8971(3)	0.0399(12)
H2A	−0.013083	0.803719	0.879695	0.048*
C3	0.0643(5)	0.6967(5)	0.9692(3)	0.0345(12)
H3A	0.016037	0.737077	1.001745	0.041*
C4	0.1562(5)	0.5928(5)	0.9943(3)	0.0312(11)
C5	0.1809(5)	0.5409(5)	1.0683(3)	0.0382(13)
C6	0.2721(5)	0.4430(6)	1.0890(3)	0.0410(13)
H6A	0.286973	0.411572	1.137757	0.049*
C7	0.3438(5)	0.3888(5)	1.0381(3)	0.0388(12)
H7A	0.405574	0.321341	1.053266	0.047*
C8	0.3245(5)	0.4337(5)	0.9662(3)	0.0336(12)
C9	0.2291(5)	0.5374(5)	0.9426(3)	0.0299(11)
C10	0.4806(4)	0.2828(5)	0.9273(3)	0.0367(12)
H10A	0.440690	0.196467	0.939820	0.044*

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Table 2 (continued)

Atom	x	y	z	U_{iso}*/U_{eq}
H10B	0.545734	0.308772	0.968444	0.044*
C11	0.5379(5)	0.2636(5)	0.8576(3)	0.0330(11)
C12	0.6645(6)	0.0669(6)	0.9214(3)	0.0484(14)
H12A	0.595909	0.003071	0.927146	0.058*
H12B	0.690000	0.117146	0.967582	0.058*
C13	0.7756(8)	−0.0113(7)	0.8989(4)	0.079(2)
H13A	0.855156	0.028612	0.923290	0.095*
H13B	0.772899	−0.109479	0.912701	0.095*
C14	0.7651(8)	0.0024(6)	0.8191(4)	0.074(2)
H14A	0.724382	−0.080262	0.794987	0.089*
H14B	0.848976	0.010953	0.805457	0.089*
C15	0.6876(5)	0.1308(5)	0.7947(3)	0.0410(13)
H15A	0.741409	0.207222	0.783283	0.049*
H15B	0.624777	0.110928	0.751341	0.049*

Source of material

The title complex was generated by reaction of 2-(5-chloroquinolin-8-yloxy)-1-(pyrrolidin-1-yl)ethanone (5 mmol) [3] with equimolar amounts of $Hg(NO_3)_2$ in acetonitrile solution. Crystals suitable for X-ray diffraction analysis were obtained by evaporating the reaction solution at room temperature.

Experimental details

The structure was solved by Direct Methods and refined with the SHELX crystallographic software package [2]. The hydrogen atoms were placed at calculated positions and refined as riding atoms with isotropic displacement parameters.

Discussion

As one of the promising systems of amide open chain ligands, quinolinyloxy acetamides can form stable complexes with various metal ions [3–5]. However, their Hg(II) complexes have been paid much less attention. In this work, the title complex from $Hg(NO_3)_2$ was synthesized and characterized by X-ray diffraction.

In the title crystal structure, the Hg(II) ion is nine-coordinated with a distorted monocapped tetragonal prism coordination geometry, involving one tridentate amide ligand and three adjacent bidentate nitrate anions, two of which also act as bridged ligands, linking the complexes into one-dimensional chains along the *b* axis. It is worth noting that O8 atom (Hg1—O8 distance being 3.012(5) Å) also participates coordination, since a longer Hg—O bond length of 3.038 Å has been reported in the literature [6]. As expected, no classical hydrogen bonds are presented in the structure.

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