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catena-Poly[[dichloridomercury(II)]-*N*′-nicotinoylnicotinohydrazide]

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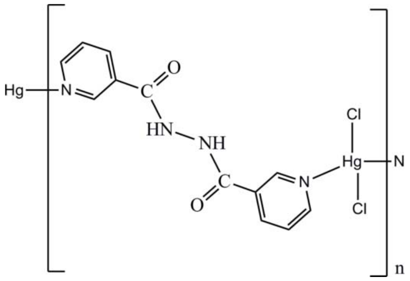
Key indicators: single-crystal X-ray study; *T* = 296 K; mean σ(C–C) = 0.004 Å; *R* factor = 0.016; *wR* factor = 0.038; data-to-parameter ratio = 13.4.

The title complex, $[HgCl_2(C_{12}H_{10}N_4O_2)]_n$, is composed of one Hg^{II} ion, one nnh ligand (nnh = *N*′-nicotinoylnicotinohydrazide) and two coordinated chloride ions. The Hg^{II} ion shows a distorted tetrahedral geometry, being surrounded by two N atoms from two nnh ligands and two chloride ions. Due to the bridging role of nnh, the Hg^{II} atoms are connected into polymeric chains along the *c* axis, which are further interlinked *via* N—H⋯O and C—H⋯Cl hydrogen-bonding interactions, forming a three-dimensional network.

Related literature

For the coordination systems of *N*-donor heterocyclic groups, see: Zhang & Chen (2010); Ma *et al.* (2005); Tao *et al.* (2010).



Experimental

Crystal data

$[HgCl_2(C_{12}H_{10}N_4O_2)]$
M_r = 513.73
Monoclinic, $P2/c$
a = 7.2514 (4) Å
b = 4.7113 (3) Å
c = 21.8591 (11) Å
β = 103.394 (2)°
V = 726.47 (7) $Å^3$
Z = 2
Mo $K\alpha$ radiation
μ = 10.97 mm^{-1}
T = 296 K
0.30 × 0.26 × 0.22 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.137, T_{max} = 0.196
3510 measured reflections
1288 independent reflections
1244 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.016
$wR(F^2)$ = 0.038
S = 1.09
1288 reflections
96 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.52 e $Å^{-3}$
$\Delta\rho_{min}$ = −0.57 e $Å^{-3}$

Table 1
Hydrogen-bond geometry (Å, °).

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
C3—H3⋯Cl1^{i}	0.93	2.81	3.558 (4)	138
N2—H2*A*⋯O1^{ii}	0.86	2.15	2.844 (3)	137

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

We acknowledge the staff of the Shanghai Institute of Materia Medica for their active cooperation in this work. We also thank the Instrument Analysis and Research Center of Nanjing University for the structural characterization.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HP2029).

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supplementary materials

Acta Cryst. (2012). E**68**, m367 [doi:10.1107/S1600536812008884]

catena-Poly[[dichloridomercury(II)]-*N*′-nicotinoylnicotinohydrazide]

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Comment

Flexible ligands containing *N*-donor heterocyclic groups, such as pyridyl, pyrazinyl, and triazolyl (see: Zhang *et al.*, 2010; Ma *et al.*, 2005; Tao *et al.*, 2010), have been widely studied in the realm of metal-organic coordination assemblies. With regard to this, *N*′-nicotinoylnicotinohydrazide (nnh), an interesting ligand with flexible spacer and multiple binding sites, has attract our attention. Herein, we report the title complex $[Hg(nnh)Cl_2]_n$, which crystallizes in the monoclinic space group *P*2/*c*, and shows a one-dimensional polymeric array and H-bonding supramolecular network.

As shown in Fig.1, the asymmetric unit of the complex is provided by a Hg^{II} center, one nnh ligand and two chloride ions. The Hg^{II} ion is tetra-coordinated to two nitrogen atoms from two nnh ligands with the Hg—N distance of 2.475 (2) Å, as well as two chloride ions with the Hg—Cl distance of 2.3405 (9) Å. The adjacent Hg centers are bridged by the nnh ligands to afford a one-dimensional zigzag chain with the Hg···Hg separation of *ca* 12.8371 (6) Å (see Fig. 2).

Notably, H-bonding interactions do play a decisive role in the crystal packing arrangement. As shown in Fig. 3, the adjacent one-dimensional arrays are linked to form a two-dimensional layer *via* N2—H2A···$O2^i$ [symmetry operation (i) = x, $1 + y$, z] hydrogen bonding between the nnh ligands from different chains. Furthermore, such two-dimensional layers are interlinked by the weak hydrogen bonds C3—H3···Cl^{ii} [symmetry operation (ii) = $-1 + x$, $-1 + y$, z] to generate a three-dimensional supramolecular network (see Fig. 4).

Experimental

A CH_3OH solution (10 ml) of nnh (24.2 mg, 0.1 mmol) was carefully layered onto an aqueous solution of $HgCl_2$ (27.1 mg, 0.1 mmol) in a straight glass tube. After evaporating the solvents slowly for *ca* one month, suitable yellow block single crystals for X-ray analysis were produced.

Refinement

All H atoms were initially located in a difference Fourier map, which were then constrained to an ideal geometry, and refined as riding atoms: C—H = 0.93 ($CH_{aromatic}$) and N—H = 0.86, with $U_{iso}(H) = 1.2U_{eq}$ (C) and $U_{iso}(H) = 1.5U_{eq}$ (N).

Computing details

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT* (Bruker, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

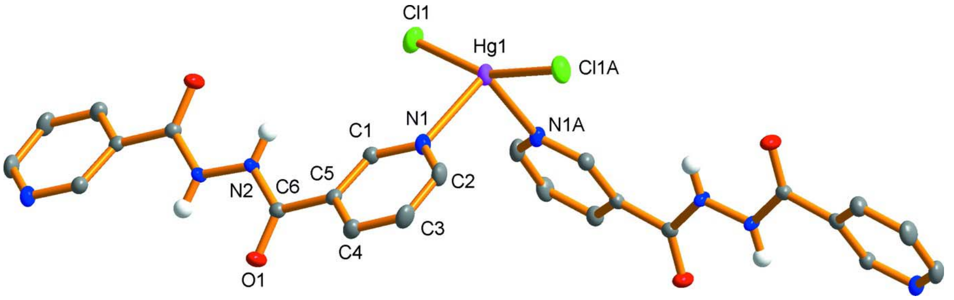

Figure 1

Coordination environment of Hg^{II} in the title complex showing displacement ellipsoids for all non-H atoms drawn at the 30% probability level. [Symmetry code (A): 1 - *x*, *y*, 3/2 - *z*.].

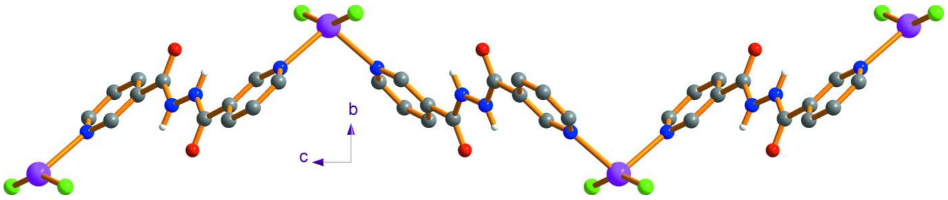

Figure 2

View of the one-dimensional chain.

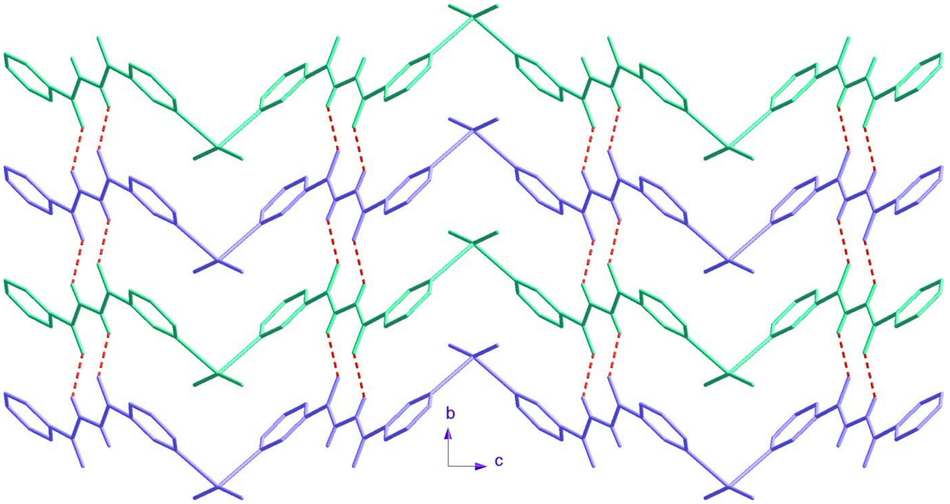

Figure 3

View of the two-dimensional layer *via* N–H···O hydrogen bonds (red dashed lines).

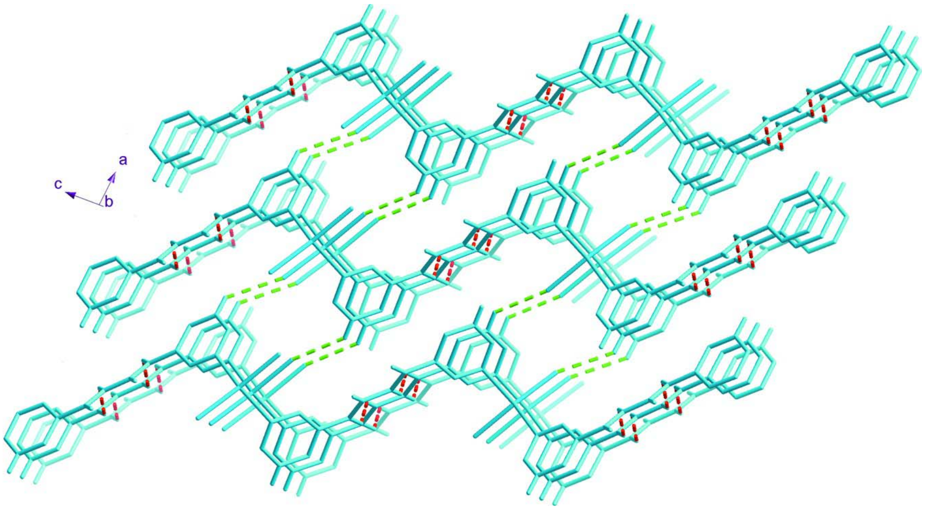

Figure 4

View of the three-dimensional network *via* C–H···Cl hydrogen bonds (green dashed lines).

***catena*-Poly[[dichloridomercury(II)]-*N*′- nicotinoylnicotinohydrazide]**

Crystal data

$[HgCl_2(C_{12}H_{10}N_4O_2)]$
$M_r = 513.73$
Monoclinic, $P2/c$
Hall symbol: -P 2yc
$a = 7.2514$ (4) Å
$b = 4.7113$ (3) Å
$c = 21.8591$ (11) Å
$\beta = 103.394$ (2)°
$V = 726.47$ (7) Å^3
$Z = 2$

$F(000) = 480$
$D_x = 2.349$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2648 reflections
$\theta = 2.9$–27.9°
$\mu = 10.97$ mm^{-1}
$T = 296$ K
BLOCK, yellow
0.30 × 0.26 × 0.22 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.137$, $T_{max} = 0.196$

3510 measured reflections
1288 independent reflections
1244 reflections with $I > 2\sigma(I)$
$R_{int} = 0.018$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.9°$
$h = -8\rightarrow8$
$k = -5\rightarrow5$
$l = -14\rightarrow26$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.016$
$wR(F^2) = 0.038$
$S = 1.09$
1288 reflections
96 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0224P)^2 + 0.0147P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.52$ e Å^{-3}
$\Delta\rho_{min} = -0.57$ e Å^{-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.

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 (Å²)

	x	*y*	*z*	$U_{\rm iso}$*/$U_{\rm eq}$
Hg1	0.5000	1.07616 (3)	0.7500	0.03638 (8)
Cl1	0.81805 (12)	1.1749 (2)	0.79628 (5)	0.0524 (2)
O1	0.7884 (3)	0.1092 (4)	0.98476 (12)	0.0385 (5)
N1	0.4508 (3)	0.7488 (5)	0.83334 (12)	0.0348 (6)
N2	0.9166 (4)	0.5412 (5)	0.97954 (13)	0.0293 (6)
H2A	0.9048	0.7096	0.9639	0.035*
C1	0.6042 (4)	0.6598 (6)	0.87486 (15)	0.0305 (6)
H1	0.7211	0.7361	0.8730	0.037*
C2	0.2825 (5)	0.6416 (8)	0.83653 (16)	0.0405 (8)
H2	0.1741	0.7054	0.8082	0.049*
C3	0.2644 (5)	0.4401 (7)	0.88032 (18)	0.0423 (8)
H3	0.1454	0.3698	0.8815	0.051*
C4	0.4239 (4)	0.3429 (7)	0.92245 (15)	0.0345 (7)
H4	0.4146	0.2023	0.9514	0.041*
C5	0.5987 (4)	0.4593 (6)	0.92072 (15)	0.0267 (6)
C6	0.7733 (4)	0.3541 (6)	0.96446 (14)	0.0264 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Hg1	0.03059 (11)	0.04571 (12)	0.02898 (11)	0.000	−0.00099 (8)	0.000
Cl1	0.0347 (4)	0.0712 (6)	0.0475 (5)	−0.0132 (4)	0.0020 (4)	−0.0076 (5)
O1	0.0319 (12)	0.0234 (10)	0.0553 (15)	0.0000 (8)	0.0000 (11)	0.0057 (9)
N1	0.0289 (13)	0.0411 (14)	0.0303 (14)	0.0040 (11)	−0.0016 (11)	−0.0001 (12)
N2	0.0235 (12)	0.0220 (11)	0.0361 (15)	−0.0008 (9)	−0.0057 (11)	0.0066 (10)
C1	0.0271 (15)	0.0304 (14)	0.0316 (16)	−0.0018 (12)	0.0017 (13)	−0.0014 (13)
C2	0.0293 (17)	0.0529 (18)	0.0331 (18)	0.0022 (14)	−0.0053 (15)	−0.0012 (15)
C3	0.0234 (17)	0.058 (2)	0.042 (2)	−0.0087 (14)	0.0019 (15)	−0.0062 (16)
C4	0.0292 (17)	0.0387 (15)	0.0339 (17)	−0.0052 (13)	0.0041 (14)	−0.0009 (14)
C5	0.0254 (15)	0.0255 (13)	0.0279 (16)	−0.0010 (11)	0.0032 (13)	−0.0054 (12)
C6	0.0251 (15)	0.0239 (13)	0.0295 (16)	0.0008 (11)	0.0051 (13)	−0.0018 (12)

Geometric parameters (Å, º)

Hg1—Cl1	2.3405 (9)	C1—C5	1.385 (5)
Hg1—Cl1^{i}	2.3405 (9)	C1—H1	0.9300
Hg1—N1^{i}	2.475 (2)	C2—C3	1.376 (5)

Hg1—N1	2.475 (2)	C2—H2	0.9300
O1—C6	1.232 (3)	C3—C4	1.379 (5)
N1—C1	1.330 (4)	C3—H3	0.9300
N1—C2	1.338 (4)	C4—C5	1.390 (4)
N2—C6	1.344 (4)	C4—H4	0.9300
N2—N2^{ii}	1.383 (5)	C5—C6	1.484 (4)
N2—H2A	0.8601		

Cl1—Hg1—Cl1^{i}	157.08 (6)	N1—C2—C3	122.1 (3)
Cl1—Hg1—N1^{i}	98.41 (6)	N1—C2—H2	118.9
Cl1^{i}—Hg1—N1^{i}	95.81 (6)	C3—C2—H2	118.9
Cl1—Hg1—N1	95.81 (6)	C2—C3—C4	119.6 (3)
Cl1^{i}—Hg1—N1	98.41 (6)	C2—C3—H3	120.2
N1^{i}—Hg1—N1	102.92 (11)	C4—C3—H3	120.2
C1—N1—C2	118.3 (3)	C3—C4—C5	118.7 (3)
C1—N1—Hg1	117.28 (19)	C3—C4—H4	120.7
C2—N1—Hg1	124.2 (2)	C5—C4—H4	120.7
C6—N2—N2^{ii}	119.0 (3)	C1—C5—C4	117.9 (3)
C6—N2—H2A	120.5	C1—C5—C6	122.1 (3)
N2^{ii}—N2—H2A	120.5	C4—C5—C6	119.9 (3)
N1—C1—C5	123.3 (3)	O1—C6—N2	121.8 (3)
N1—C1—H1	118.3	O1—C6—C5	122.4 (3)
C5—C1—H1	118.3	N2—C6—C5	115.8 (2)

Cl1—Hg1—N1—C1	−12.5 (2)	C2—C3—C4—C5	2.1 (5)
Cl1^{i}—Hg1—N1—C1	−174.5 (2)	N1—C1—C5—C4	1.1 (5)
N1^{i}—Hg1—N1—C1	87.6 (2)	N1—C1—C5—C6	177.0 (3)
Cl1—Hg1—N1—C2	172.4 (2)	C3—C4—C5—C1	−2.5 (5)
Cl1^{i}—Hg1—N1—C2	10.4 (3)	C3—C4—C5—C6	−178.5 (3)
N1^{i}—Hg1—N1—C2	−87.6 (3)	N2^{ii}—N2—C6—O1	−2.0 (5)
C2—N1—C1—C5	0.8 (5)	N2^{ii}—N2—C6—C5	179.5 (3)
Hg1—N1—C1—C5	−174.6 (2)	C1—C5—C6—O1	−147.0 (3)
C1—N1—C2—C3	−1.3 (5)	C4—C5—C6—O1	28.8 (4)
Hg1—N1—C2—C3	173.8 (3)	C1—C5—C6—N2	31.5 (4)
N1—C2—C3—C4	−0.2 (5)	C4—C5—C6—N2	−152.7 (3)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···Cl1^{iii}	0.93	2.81	3.558 (4)	138
N2—H2*A*···O1^{iv}	0.86	2.15	2.844 (3)	137

Symmetry codes: (iii) $x-1, y-1, z$; (iv) $x, y+1, z$.