IUCrData

ISSN 2414-3146

catena-Poly[[μ_2-4,4′-bis(pyridin-3-ylethynyl)-1,1′-biphenyl-κ^2N:N']bis(μ_2-thiocyanato-κ^2N:S)-bis(thiocyanato-κS)dimercury(II)]

Shuzhi Tan,* Leili Liu and Yongli Du

School of Chemistry and Pharmaceutical Engineering, Qilu University of Technology, Jinan, Shandong 250353, People's Republic of China. *Correspondence e-mail: cyrstalclear@126.com

Received 13 December 2016
Accepted 12 January 2017

Edited by S. Bernès, Benemérita Universidad Autónoma de Puebla, México

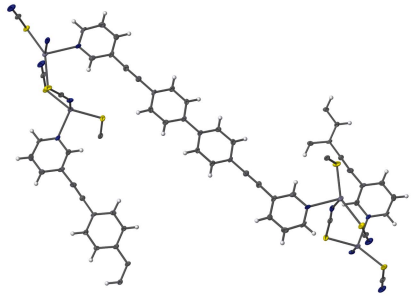
Keywords: crystal structure; inorganic polymer; thiocyanate.

CCDC reference: 1526974

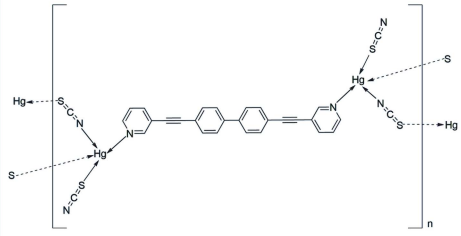
Structural data: full structural data are available from iucrdata.iucr.org

In the title polymer, $[Hg_2(SCN)_4(C_{26}H_{16}N_2)]_n$, the two equivalent Hg^{II} atoms are coordinated by one N atom of a bridging 4,4′-bis(pyridin-3-ylethynyl)-1,1′-biphenyl ligand, two S atoms of two thiocyanates and one N atom of a thiocyanate, giving rise to a distored tetrahedral coordination environment. Two thiocyanate ligands bridge symmetry-related metal atoms to form a polymeric chain extending parallel to [001], and another bridging mode is accomplished by the organic ligand that is located about an inversion centre. The dihedral angle between the coordinating pyridine ring and the benzene ring is 11.4 (2)°, and the two coordinating pyridine rings in the organic ligand are parallel by symmetry. The point group of the ligand in the compound is thus close to C_{2h}. The result of the mode of the organic ligands is the formation of zigzag sheets connected *via* bridging thiocyanate ligands.

3D view



Chemical scheme



Structure description

Recently, coordination polymers (CPs) have attracted much attention due to their fascinating structures as well as their potential applications in gas storage and separation, heterogeneous catalysis, proton conductivity, and luminescent sensors, *etc*. Organic ligands play a key role in the construction of CPs with various structures and topologies with pyridine-based ligands being widely used. A mercury-based coordination polymer was described by Wang *et al.* (2014).

In this work, an angular pyridine-based ligand, 4,4′-bis(pyridin-3-ylethynyl)-1,1′-biphenyl (*L*) was synthesized and employed to react with $Hg(SCN)_2$ to afford the title complex, $[Hg_2(SCN)_4(L)]_n$. The Hg^{II} atom is coordinated by one N atom of an *L* ligand, two S atoms of two thiocyanate ligands (one bridging, one terminal) and one N atom of

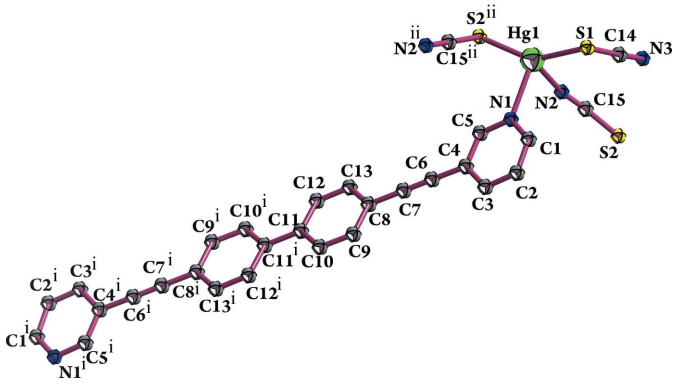


Figure 1
The coordination mode of the title complex, with displacement ellipsoids drawn at the 50% probability level. All H atoms have been omitted for clarity. [Symmetry codes: (i) $-2-x, 1-y, -z$; (ii) $x, -y+\frac{1}{2}, z-\frac{1}{2}$.]

the another bridging thiocyanate ligand, in a distorted tetrahedral environment (Table 1 and Fig. 1). The dihedral angle between the coordinating pyridine ring and the benzene ring is 11.4 (2)°, and the two coordinating pyridine rings are parallel, by symmetry. The formed inorganic $[Hg(SCN)_2]_n$ chains are bridged by the organic ligands into a three-dimensional network, whereby the organic ligands are arranged in zigzag sheets approximately parallel to (010) (Fig. 2). Within an organic sheet π–π interactions between nearly parallel aligned pyridine and benzene rings of neighbouring ligands are evident, with a centroid-to-centroid distance of 3.655 (3) Å.

Synthesis and crystallization

The organic ligand *L*, 4,4′-bis(pyridin-3-ylethynyl)-1,1′-biphenyl, was synthesized following the reported procedure (Kaae *et al.*, 2012). 3 ml of a methanol solution of $Hg(SCN)_2$ (0.1 mmol, 31 mg) was layered upon 3 ml of a chloroform solution of *L* (0.2 mmol, 70 mg). After 4 d, yellow crystals of the title complex suitable for X-ray analysis were obtained.

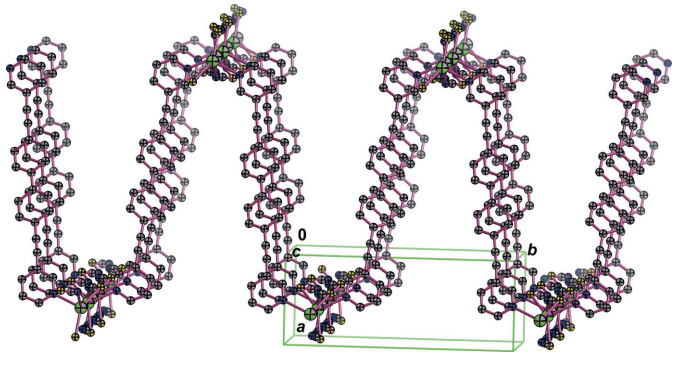


Figure 2
The zigzag sheets of the complex, viewed down the *c* axis, with displacement ellipsoids drawn at the 50% probability level. All H atoms have been omitted for clarity.

Table 1
Selected geometric parameters (Å, °).

Hg1—N1	2.392 (4)	Hg1—S2^{i}	2.4325 (13)
Hg1—S1	2.4170 (13)	Hg1—N2	2.568 (5)
N1—Hg1—S1	109.28 (10)	N1—Hg1—N2	84.04 (13)
N1—Hg1—S2^{i}	99.19 (10)	S1—Hg1—N2	98.29 (10)
S1—Hg1—S2^{i}	148.61 (5)	S2^{i}—Hg1—N2	97.50 (11)

Symmetry code: (i) $x, -y+\frac{1}{2}, z-\frac{1}{2}$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Hg_2(SCN)_4(C_{26}H_{16}N_2)]$
M_r	989.9
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, *b*, *c* (Å)	6.9175 (5), 17.6267 (13), 12.0029 (9)
β (°)	91.017 (1)
V (Å^3)	1463.32 (19)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	10.80
Crystal size (mm)	0.20 × 0.18 × 0.18
Data collection	
Diffractometer	Bruker *SMART* 1000 CCD area-detector diffractometer
Absorption correction	Multi-scan (*SADABS*; Bruker, 1998)
T_{min}, T_{max}	0.221, 0.247
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7862, 2726, 2275
R_{int}	0.030
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.606
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.028, 0.062, 1.02
No. of reflections	2726
No. of parameters	190
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.52, −0.78

Computer programs: *SMART* and *SAINT* (Bruker, 1998), *SHELXS97* and *SHELXTL* (Sheldrick, 2008), *SHELXL2016/6* (Sheldrick, 2015).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The maximum and minimum residual electron density peaks of 2.15 and 1.73 e Å^{-3}, respectively, are located 0.93 and 1.00 Å from the Hg atom.

Acknowledgements

The authors thank Qilu University of Technology for supporting this work.

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full crystallographic data

IUCrData (2017). **2**, x170059 [https://doi.org/10.1107/S2414314617000591]

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***catena*-Poly[[μ_2-4,4′-bis(pyridin-3-ylethynyl)-1,1′-biphenyl-κ^2N:N']bis(μ_2-thiocyanato-κ^2N:S)bis(thiocyanato-κS)dimercury(II)]**

Crystal data

$[Hg_2(SCN)_4(C_{26}H_{16}N_2)]$
M_r = 989.9
Monoclinic, $P2_1/c$
a = 6.9175 (5) Å
b = 17.6267 (13) Å
c = 12.0029 (9) Å
β = 91.017 (1)°
V = 1463.32 (19) Å^3
Z = 2
$F(000)$ = 924
D_x = 2.247 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2275 reflections
θ = 2.1–25.5°
μ = 10.80 mm^{-1}
T = 100 K
Block, yellow
0.20 × 0.18 × 0.18 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
ω and phi scans
Absorption correction: multi-scan (SADABS; Bruker, 1998)
T_{min} = 0.221, T_{max} = 0.247
7862 measured reflections
2726 independent reflections
2275 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 25.5°, θ_{min} = 2.1°
h = −8→8
k = −20→21
l = −10→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.062
S = 1.02
2726 reflections
190 parameters
0 restraints
0 constraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0265P)^2 + 1.8001P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.78 e Å^{-3}

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

	x	y	z	U_{iso}*/U_{eq}
Hg1	0.34026 (3)	0.25411 (2)	0.44910 (2)	0.01732 (8)
S1	0.65961 (18)	0.27179 (8)	0.52991 (12)	0.0205 (3)
S2	0.1157 (2)	0.32566 (8)	0.84385 (12)	0.0227 (3)

N1	0.1994 (6)	0.3753 (2)	0.4098 (3)	0.0156 (9)
N2	0.1456 (6)	0.2626 (2)	0.6289 (4)	0.0192 (10)
N3	0.5993 (7)	0.2468 (3)	0.7608 (4)	0.0295 (12)
C1	0.3013 (7)	0.4384 (3)	0.4306 (5)	0.0204 (12)
H1	0.425505	0.433605	0.464884	0.025*
C2	0.2349 (8)	0.5101 (3)	0.4046 (5)	0.0248 (13)
H2	0.311575	0.553457	0.421443	0.030*
C3	0.0562 (7)	0.5181 (3)	0.3540 (5)	0.0214 (12)
H3	0.007957	0.567035	0.335333	0.026*
C4	−0.0549 (7)	0.4526 (3)	0.3300 (4)	0.0163 (11)
C5	0.0234 (7)	0.3833 (3)	0.3607 (4)	0.0182 (11)
H5	−0.050779	0.338861	0.346461	0.022*
C6	−0.2388 (7)	0.4581 (3)	0.2727 (4)	0.0182 (12)
C7	−0.3830 (7)	0.4664 (3)	0.2206 (5)	0.0189 (12)
C8	−0.5611 (7)	0.4759 (3)	0.1569 (4)	0.0143 (11)
C9	−0.6090 (7)	0.5459 (3)	0.1106 (5)	0.0185 (12)
H9	−0.524889	0.587946	0.121710	0.022*
C10	−0.7775 (7)	0.5550 (3)	0.0487 (4)	0.0147 (11)
H10	−0.805817	0.602942	0.016040	0.018*
C11	−0.9079 (7)	0.4947 (3)	0.0330 (4)	0.0145 (11)
C12	−0.8575 (7)	0.4249 (3)	0.0807 (4)	0.0159 (11)
H12	−0.943342	0.383226	0.071779	0.019*
C13	−0.6881 (7)	0.4148 (3)	0.1398 (4)	0.0175 (11)
H13	−0.656548	0.366182	0.169164	0.021*
C14	0.6192 (8)	0.2577 (3)	0.6661 (5)	0.0211 (12)
C15	0.1390 (7)	0.2870 (3)	0.7177 (5)	0.0169 (11)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Hg1	0.01973 (12)	0.01986 (12)	0.01214 (12)	0.00123 (9)	−0.00573 (8)	0.00026 (9)
S1	0.0173 (6)	0.0301 (7)	0.0139 (7)	−0.0010 (6)	−0.0030 (6)	0.0026 (6)
S2	0.0288 (7)	0.0258 (7)	0.0135 (7)	0.0112 (6)	−0.0051 (6)	−0.0039 (6)
N1	0.015 (2)	0.021 (2)	0.010 (2)	−0.0006 (17)	−0.0049 (19)	−0.0024 (18)
N2	0.019 (2)	0.022 (2)	0.016 (3)	0.0052 (18)	−0.004 (2)	0.003 (2)
N3	0.027 (3)	0.047 (3)	0.014 (3)	0.001 (2)	−0.007 (2)	−0.001 (2)
C1	0.013 (3)	0.031 (3)	0.017 (3)	0.000 (2)	−0.009 (2)	0.002 (2)
C2	0.026 (3)	0.022 (3)	0.026 (4)	−0.006 (2)	−0.004 (3)	−0.004 (2)
C3	0.024 (3)	0.018 (3)	0.022 (3)	0.003 (2)	−0.006 (3)	0.000 (2)
C4	0.014 (3)	0.027 (3)	0.008 (3)	0.005 (2)	−0.001 (2)	0.002 (2)
C5	0.017 (3)	0.024 (3)	0.013 (3)	−0.004 (2)	−0.002 (2)	−0.001 (2)
C6	0.020 (3)	0.022 (3)	0.013 (3)	0.003 (2)	0.001 (2)	0.004 (2)
C7	0.017 (3)	0.021 (3)	0.018 (3)	0.000 (2)	−0.002 (2)	0.001 (2)
C8	0.010 (2)	0.023 (3)	0.010 (3)	0.0043 (19)	−0.002 (2)	0.000 (2)
C9	0.012 (3)	0.020 (3)	0.023 (3)	0.000 (2)	−0.004 (2)	0.001 (2)
C10	0.016 (2)	0.017 (2)	0.011 (3)	0.005 (2)	0.001 (2)	0.001 (2)
C11	0.012 (2)	0.021 (3)	0.010 (3)	0.002 (2)	−0.001 (2)	0.000 (2)
C12	0.017 (3)	0.020 (3)	0.010 (3)	−0.001 (2)	−0.001 (2)	−0.001 (2)

C13	0.022 (3)	0.017 (2)	0.013 (3)	0.005 (2)	0.000 (2)	0.001 (2)
C14	0.015 (3)	0.027 (3)	0.021 (3)	0.000 (2)	−0.006 (2)	−0.003 (2)
C15	0.012 (3)	0.021 (3)	0.018 (3)	0.000 (2)	−0.002 (2)	0.003 (2)

Geometric parameters (Å, º)

Hg1—N1	2.392 (4)	C4—C5	1.384 (7)
Hg1—S1	2.4170 (13)	C4—C6	1.438 (7)
Hg1—S2^{i}	2.4325 (13)	C5—H5	0.9500
Hg1—N2	2.568 (5)	C6—C7	1.178 (7)
S1—C14	1.682 (6)	C7—C8	1.448 (7)
S2—C15	1.671 (6)	C8—C9	1.392 (7)
N1—C1	1.338 (6)	C8—C13	1.402 (7)
N1—C5	1.351 (6)	C9—C10	1.381 (7)
N2—C15	1.151 (7)	C9—H9	0.9500
N3—C14	1.163 (8)	C10—C11	1.404 (7)
C1—C2	1.378 (7)	C10—H10	0.9500
C1—H1	0.9500	C11—C12	1.398 (7)
C2—C3	1.375 (7)	C11—C11^{ii}	1.500 (9)
C2—H2	0.9500	C12—C13	1.371 (7)
C3—C4	1.413 (7)	C12—H12	0.9500
C3—H3	0.9500	C13—H13	0.9500
N1—Hg1—S1	109.28 (10)	N1—C5—H5	118.2
N1—Hg1—S2^{i}	99.19 (10)	C4—C5—H5	118.2
S1—Hg1—S2^{i}	148.61 (5)	C7—C6—C4	175.0 (6)
N1—Hg1—N2	84.04 (13)	C6—C7—C8	179.4 (6)
S1—Hg1—N2	98.29 (10)	C9—C8—C13	118.6 (4)
S2^{i}—Hg1—N2	97.50 (11)	C9—C8—C7	120.5 (4)
C14—S1—Hg1	101.81 (19)	C13—C8—C7	120.9 (4)
C15—S2—Hg1^{iii}	99.43 (18)	C10—C9—C8	120.7 (5)
C1—N1—C5	117.6 (4)	C10—C9—H9	119.6
C1—N1—Hg1	119.6 (3)	C8—C9—H9	119.6
C5—N1—Hg1	122.7 (3)	C9—C10—C11	121.2 (5)
C15—N2—Hg1	146.1 (4)	C9—C10—H10	119.4
N1—C1—C2	123.2 (5)	C11—C10—H10	119.4
N1—C1—H1	118.4	C12—C11—C10	117.1 (4)
C2—C1—H1	118.4	C12—C11—C11^{ii}	121.9 (6)
C3—C2—C1	119.2 (5)	C10—C11—C11^{ii}	121.0 (6)
C3—C2—H2	120.4	C13—C12—C11	122.1 (5)
C1—C2—H2	120.4	C13—C12—H12	118.9
C2—C3—C4	119.2 (5)	C11—C12—H12	118.9
C2—C3—H3	120.4	C12—C13—C8	120.2 (5)
C4—C3—H3	120.4	C12—C13—H13	119.9
C5—C4—C3	117.3 (5)	C8—C13—H13	119.9
C5—C4—C6	121.7 (5)	N3—C14—S1	177.1 (5)
C3—C4—C6	121.0 (5)	N2—C15—S2	176.1 (5)
N1—C5—C4	123.6 (5)		

C5—N1—C1—C2	0.2 (8)	C13—C8—C9—C10	−0.3 (8)
Hg1—N1—C1—C2	176.3 (4)	C7—C8—C9—C10	179.2 (5)
N1—C1—C2—C3	−0.6 (9)	C8—C9—C10—C11	1.7 (8)
C1—C2—C3—C4	0.1 (9)	C9—C10—C11—C12	−1.4 (8)
C2—C3—C4—C5	0.8 (8)	C9—C10—C11—C11^{ii}	179.1 (6)
C2—C3—C4—C6	−177.2 (5)	C10—C11—C12—C13	−0.4 (8)
C1—N1—C5—C4	0.8 (8)	C11^{ii}—C11—C12—C13	179.1 (6)
Hg1—N1—C5—C4	−175.2 (4)	C11—C12—C13—C8	1.8 (8)
C3—C4—C5—N1	−1.3 (8)	C9—C8—C13—C12	−1.5 (8)
C6—C4—C5—N1	176.8 (5)	C7—C8—C13—C12	179.1 (5)

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