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The crystal structure of *catena*-poly[chlorido-(μ_2 -5-methyl-1,3,4-thiadiazole-2-thiolato- κ^2 S:N)mercury(II)], $C_3H_3ClHgN_2S_2$

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.17 × 0.09 × 0.05 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	20.7 mm ⁻¹
Diffractometer, scan mode:	CCD Area Detector, φ and ω
$\theta_{\max}$, completeness:	28.3°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	5143, 1849, 0.053
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1354
$N(\text{param})_{\text{refined}}$:	84
Programs:	Bruker [1], Olex2 [2], SHELX [3]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Hg1	1.05409(4)	1.19998(15)	0.01403(8)	0.0499(2)
Cl1	1.1325(3)	1.5467(15)	0.1282(6)	0.0642(14)
S1	0.8364(3)	0.5636(13)	0.0571(4)	0.0497(12)
S2	0.9645(3)	0.8633(13)	−0.0819(5)	0.0513(13)
N1	0.9365(10)	0.869(4)	0.1863(16)	0.050(4)
N2	0.8866(10)	0.760(4)	0.2774(16)	0.051(4)
C1	0.9193(13)	0.776(4)	0.0618(18)	0.045(4)
C2	0.8300(11)	0.601(4)	0.2295(18)	0.042(4)
C3	0.7713(13)	0.476(5)	0.311(2)	0.060(6)
H3A	0.774175	0.241065	0.315337	0.090*
H3B	0.726778	0.538356	0.271805	0.090*
H3C	0.774689	0.565630	0.398478	0.090*

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Abstract

$C_3H_3ClHgN_2S_2$, orthorhombic, $Pna2_1$ (no. 33), $a = 18.794(8)$ Å, $b = 4.0798(17)$ Å, $c = 10.093(4)$ Å, $V = 773.8(6)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0437$, $wR_{\text{ref}}(F^2) = 0.1024$, $T = 291(2)$ K.

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The crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of materials

To a acetonitrile solution (15 mL) of 2-mercapto-5-methyl-1,3,4-thiadiazole (McMT) (1 mmol) was added an acetonitrile solution of mercury(II) chloride (1 mmol) and stirred for 15 min which yielded a white suspension. The precipitate was filtered off and washed with acetonitrile to give a pure powder in a yield of 79%. Elem. anal. calcd. for $C_3H_3ClHgN_2S_2$ (%): C, 9.81%; H, 0.82%; N, 7.63%;

S, 17.46%. Found(%): C, 9.78%; H, 0.84%; N, 7.66%; S, 17.45%. A sample of the title complex was dissolved in acetonitrile. Upon slow evaporation at room temperature, colorless, block-shaped crystals were obtained after several days.

Experimental details

All hydrogen atoms were placed at calculated positions and refined with a riding model, with $d(C-H) = 0.96$ Å. U_{iso} parameters of hydrogen atoms were set to $1.5U_{\text{eq}}(C)$ for methyl groups. The highest peak and the deepest hole in the difference Fourier map are 1.789 e Å^{-3} and -1.745 e Å^{-3} , respectively.

Comment

Mercapto-triazoles and derivatives are important heterocyclic compounds and have been extensively studied due to their applications as pharmacologically significant scaffolds of anti-cancer, anti-depressant, anti-oxidant, anti-convulsant,

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anti-microbial, enzyme inhibitors and anti-inflammatory drugs [4–7]. They are also used as metal chelating agents, corrosion inhibitors, antiwear agents and cross-linkers for polymers [8–10]. In our previous study, silver(I) and mercury (II) complexes with 1,3,4-thiadiazole were structurally characterized [11, 12]. McMT are significant ligands which are able to bridge metal centers [13, 14]. Because of the high toxicity and severe effects on living organisms, Hg²⁺ has drawn the attention of researchers. It can be used in the manufacture of industrial products and can bind to many ligands and complexes present in organisms [15–17]. Based on these considerations Hg(II) complexes of McMT, may be applied for the removal of mercury.

The crystal structures of the title compound show that all Hg(II) ions are equivalent and Hg(II) is three coordinated with one chloride anion, one nitrogen atom and one sulfur atom of two adjacent McMTs, respectively. The bond lengths of Hg–Cl, Hg–S and Hg–N are 2.346(4) Å, 2.380(4) Å, and 2.650(11) Å, showing strong to weak interactions between Hg(II) and the ligand. The involving Hg atoms bond angles of Cl(1)–Hg(1)–S(2), Cl(1)–Hg(1)–N(2) and S(2)–Hg(1)–N(2) are 73.14(15)°, 98.4(3)° and 87.9(3)°, respectively. The thiadiazole ring is almost planar and the largest torsion angle within the five-membered ring is –176.7(9)°. For each McMT, the bond lengths N1–C1 and N2–C2 are 1.356(17) Å and 1.330(17) Å, which indicate pure double character [18]. In addition, a weak hydrogen bond occurs between coordinated Cl atom and another H (thiadiazole moiety) (2.831 Å for Cl1···H3B).

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