Crystal structure of dichloro(pyridine-2-aldoxime-*N*,*N'*)mercury(II), $HgCl_2(NC_5H_4CHNOH)$

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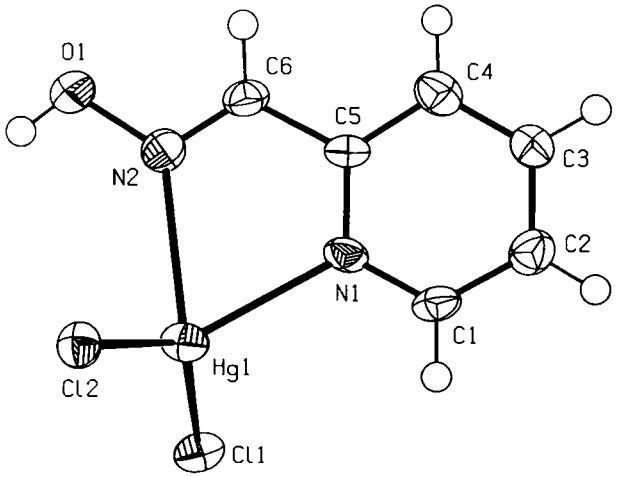

Abstract

$C_6H_6Cl_2HgN_2O$, triclinic, $P\bar{1}$ (no. 2), $a = 3.8750(1)$ Å, $b = 8.7240(3)$ Å, $c = 13.9420(5)$ Å, $\alpha = 107.06(5)°$, $\beta = 95.90(5)°$, $\gamma = 95.22(5)°$, $V = 444.5$ Å^3, $Z = 2$, $R_{gt}(F) = 0.044$, $wR_{ref}(F^2) = 0.129$, $T = 173$ K.

Source of material

Dichloro(pyridine-2-carbaldoxime)mercury(II) was formed by reacting of pyridine-2-carbaldoxime as ligand (0.34 g, 2.7 mmol) with mercury(II) chloride (0.4 g, 1.4 mmol) in methanol (4 ml) at 45 °C. After a week colorless crystals were obtained (m.p. 210 °C).

Discussion

The title compound, $HgCl_2[C_5NH_4]CHNOH$, exists in the solid state with the Hg atom linked by bridging N atoms. Our attention was drawn to potentially coordinating pyridine-2-carbaldoxime ligand, recorded initially as forming mononuclear complex manganese(II) and zinc(II) salts [1]. In the present research, a 1:1 mercury(II) chloride/pyridine-2-carbaldoxime complex was synthesized. The pyridine-2-carbaldoxime ligand in this complex is coordinating via N atoms. There is a significant difference between Hg—N1 (2.363(6) Å) and Hg—N2 (2.524(7) Å) bond lengths. However, the distances are in the range of 2.106 Å to 2.800 Å reported for Hg—N bond lengths [2-5]. The valence bond angles around the metal atom are 101.4(2)°, 93.0(2)°, 67.5(2)° and 134.10(7)° respected to N1–Hg–Cl1, N2–Hg–Cl2, N1–Hg–N2 and Cl1–Hg–Cl2. The complex is insoluble in dichloromethane, chloroform, water, acetone and acetonitrile, which indicates that it can be a good tool for removing mercury from industrial residual.

Table 1. Data collection and handling.

Crystal:	colorless prism, size 0.05 × 0.05 × 0.05 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	178.62 cm^{-1}
Diffractometer, scan mode:	Nonius KappaCCD, φ
$2\theta_{max}$:	60.1°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	2598, 2597
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 2370
$N(param)_{refined}$:	110
Programs:	SIR92 [6], SHELXL-97 [7], PLATON [8]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(1O)	2*i*	0.1501	0.8056	0.5202	0.045
H(1)	2*i*	1.0544	0.8453	0.9257	0.025
H(2)	2*i*	1.1710	0.6085	0.9617	0.029
H(3)	2*i*	0.9484	0.3586	0.8437	0.028
H(4)	2*i*	0.6170	0.3504	0.6905	0.029
H(6)	2*i*	0.3489	0.4975	0.5791	0.026

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Hg(1)	2*i*	0.68096(7)	0.98022(3)	0.75093(2)	0.0232(2)	0.0181(2)	0.0213(2)	0.0008(1)	0.0049(1)	0.0031(1)
Cl(1)	2*i*	0.3869(5)	1.1181(2)	0.8895(1)	0.0180(7)	0.0232(8)	0.0193(8)	0.0011(6)	0.0028(6)	0.0010(6)
Cl(2)	2*i*	0.9983(5)	1.0659(2)	0.6315(1)	0.0228(8)	0.0245(9)	0.0213(8)	0.0048(6)	0.0049(6)	0.0077(7)
O(1)	2*i*	0.184(2)	0.7136(8)	0.5239(5)	0.034(3)	0.023(3)	0.027(3)	0.003(2)	−0.010(3)	0.004(2)
N(1)	2*i*	0.777(2)	0.7414(8)	0.7914(5)	0.017(3)	0.013(3)	0.024(3)	−0.003(2)	0.000(2)	0.004(2)
N(2)	2*i*	0.372(2)	0.7291(9)	0.6174(5)	0.017(3)	0.022(3)	0.025(3)	0.000(2)	−0.002(2)	0.007(3)

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Table 3. Continued.

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(1)	2*i*	0.965(2)	0.7438(9)	0.8775(6)	0.023(3)	0.019(3)	0.016(3)	–0.006(3)	0.002(3)	0.002(3)
C(2)	2*i*	1.035(2)	0.603(1)	0.8997(6)	0.024(4)	0.026(4)	0.023(4)	–0.003(3)	–0.001(3)	0.009(3)
C(3)	2*i*	0.904(2)	0.456(1)	0.8301(6)	0.026(4)	0.019(3)	0.025(4)	0.001(3)	0.001(3)	0.008(3)
C(4)	2*i*	0.707(2)	0.451(1)	0.7400(7)	0.023(4)	0.020(3)	0.029(4)	0.001(3)	0.004(3)	0.008(3)
C(5)	2*i*	0.646(2)	0.5967(9)	0.7245(6)	0.017(3)	0.014(3)	0.017(3)	0.000(2)	0.003(2)	0.000(2)
C(6)	2*i*	0.436(2)	0.597(1)	0.6300(6)	0.023(3)	0.019(3)	0.017(3)	0.003(3)	0.001(3)	0.000(3)

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