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Crystal structure of bis{1-[(benzotriazol-1-yl)methyl]-1*H*-1,3-(2-methyl-imidazol)}dichloridomercury(II), [Hg(C₁₁H₁₁N₅)₂Cl₂], C₂₂H₂₂N₁₀Cl₂Hg

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.18 × 0.15 × 0.14 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	6.28 mm ⁻¹
Diffractometer, scan mode:	Xcalibur, ω
$\theta_{\max}$, completeness:	26.4°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	10,530, 5193, 0.033
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2\sigma(I_{\text{obs}})$, 4361
$N(\text{param})_{\text{refined}}$:	318
Programs:	CrysAlis ^{PRO} [1], Olex2 [2], SHELX [3]

Abstract

C₂₂H₂₂N₁₀Cl₂Hg, triclinic, $P\bar{1}$ (no. 2), $a = 8.2034(4)$ Å, $b = 12.7859(7)$ Å, $c = 13.5026(7)$ Å, $\alpha = 66.069(5)^\circ$, $\beta = 79.964(4)^\circ$, $\gamma = 84.465(4)^\circ$, $V = 1274.18(12)$ Å³, $Z = 2$, $R_{\text{gt}}(F) = 0.0372$, $\omega R_{\text{ref}}(F^2) = 0.0670$, $T = 291.15$ K.

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Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

A methanol solution (4 mL) of KSCN (0.1 mmol) was added dropwise into a methanol solution (2 mL) of HgCl₂ (0.05 mmol), giving a clear solution. 1-[(Benzotriazol-1-yl)methyl]-1*H*-1,3-(2-methyl-imidazol) (0.1 mmol) in 4 mL of methanol was added dropwise to the above mixture solution. The resulting solution was left at room temperature. After three days, good quality colorless crystals were obtained from the solution and dried in air.

Experimental details

H atoms were generated geometrically, with C–H = 0.96, 0.97 and 0.93 Å for methyl, methylene and aromatic H,

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

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}
Hg1	0.75903 (2)	0.23921 (2)	−0.03776 (2)	0.04653 (8)
Cl1	0.51595 (15)	0.20105 (12)	−0.09669 (11)	0.0546 (3)
Cl2	0.97050 (17)	0.34967 (13)	−0.18343 (11)	0.0646 (4)
N1	0.6879 (5)	0.3646 (3)	0.0480 (3)	0.0427 (10)
N2	0.5670 (5)	0.4516 (3)	0.1524 (3)	0.0407 (10)
N3	0.4635 (5)	0.4093 (3)	0.3430 (3)	0.0403 (9)
N4	0.3462 (5)	0.3317 (4)	0.4074 (4)	0.0552 (12)
N5	0.3781 (6)	0.2872 (4)	0.5063 (4)	0.0596 (12)
N6	0.8300 (4)	0.0788 (3)	0.0963 (3)	0.0419 (10)
N7	0.9656 (4)	−0.0527 (3)	0.2156 (3)	0.0394 (9)
N8	1.1641 (5)	−0.0810 (3)	0.3403 (3)	0.0412 (10)
N9	1.2991 (5)	−0.0137 (4)	0.2996 (4)	0.0551 (12)
N10	1.3520 (5)	−0.0027 (4)	0.3802 (4)	0.0578 (12)
C1	0.7755 (6)	0.4586 (5)	0.0263 (4)	0.0536 (14)
H1	0.870775	0.481753	−0.024727	0.064*
C2	0.7022 (7)	0.5131 (5)	0.0905 (4)	0.0540 (14)
H2	0.737038	0.579388	0.092161	0.065*
C3	0.5620 (6)	0.3603 (4)	0.1247 (4)	0.0386 (11)
C4	0.4334 (6)	0.2724 (4)	0.1750 (4)	0.0570 (14)
H4A	0.433455	0.231296	0.129207	0.086*
H4B	0.326797	0.308895	0.182405	0.086*
H4C	0.456714	0.220019	0.245961	0.086*
C5	0.4461 (6)	0.4803 (4)	0.2312 (4)	0.0431 (12)
H5A	0.458008	0.559612	0.218578	0.052*
H5B	0.335570	0.472533	0.219077	0.052*
C6	0.5743 (6)	0.4136 (4)	0.4060 (4)	0.0388 (11)
C7	0.5196 (7)	0.3353 (4)	0.5094 (4)	0.0482 (13)
C8	0.6000 (8)	0.3217 (5)	0.5983 (5)	0.0644 (17)
H8	0.563890	0.270078	0.669117	0.077*
C9	0.7317 (9)	0.3874 (6)	0.5755 (6)	0.075 (2)
H9	0.786547	0.381177	0.632499	0.090*
C10	0.7892 (7)	0.4648 (6)	0.4691 (6)	0.0713 (18)
H10	0.881818	0.507186	0.457712	0.086*
C11	0.7128 (6)	0.4800 (5)	0.3811 (5)	0.0554 (14)
H11	0.750594	0.530861	0.310227	0.066*
C12	0.7186 (6)	0.0015 (4)	0.1744 (4)	0.0469 (13)
H12	0.604564	0.005875	0.175301	0.056*
C13	0.7991 (6)	−0.0796 (4)	0.2477 (4)	0.0478 (13)
H13	0.753639	−0.141831	0.308251	0.057*
C14	0.9783 (5)	0.0437 (4)	0.1235 (4)	0.0387 (11)
C15	1.1363 (6)	0.1007 (5)	0.0630 (4)	0.0588 (15)
H15A	1.118746	0.155614	−0.008352	0.088*
H15B	1.218151	0.044361	0.055460	0.088*
H15C	1.174034	0.138845	0.102700	0.088*
C16	1.1030 (6)	−0.1225 (4)	0.2687 (4)	0.0461 (13)
H16A	1.066648	−0.200279	0.311134	0.055*
H16B	1.193273	−0.124625	0.212581	0.055*
C17	1.1330 (5)	−0.1164 (4)	0.4506 (4)	0.0383 (11)
C18	1.2528 (6)	−0.0665 (4)	0.4764 (4)	0.0439 (12)
C19	1.2653 (7)	−0.0869 (5)	0.5845 (5)	0.0608 (16)
H19	1.345950	−0.053411	0.601844	0.073*
C20	1.1526 (7)	−0.1587 (6)	0.6633 (5)	0.0699 (18)
H20	1.157755	−0.175165	0.736369	0.084*
C21	1.0309 (7)	−0.2080 (5)	0.6388 (5)	0.0696 (17)

Table 2: (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}
H21	0.956250	−0.255624	0.695713	0.084*
C22	1.0170 (6)	−0.1887 (5)	0.5319 (5)	0.0566 (15)
H22	0.935149	−0.221824	0.515340	0.068*

respectively, and constrained to ride on their parent atoms with $U_{\text{iso}}(\text{H}) = x$ times $U_{\text{eq}}(\text{C})$, where $x = 1.5$ for methyl H and $x = 1.2$ for all other H atoms.

Comment

The multidentate *N*-heterocyclic compounds containing rich coordination sites and presenting various coordination modes, are often employed to produce coordination polymers [4–9]. In recent years, our group synthesized *N*-heterocyclic compounds based on 1-[(benzotriazol-1-yl)methyl]-1-*H*-1,3-(2-methyl-imidazol)(bmi), and studied its coordination behavior with metal ions, obtaining a series of coordination compounds [10–16]. Furthermore, to study the effect of subsidiary ligands on the coordination behavior of this ligand, we used bmi to react with metal salts in the presence of KSCN, and also obtained a series of complexes. Single crystal X-ray diffraction indicated that the ion SCN[−] coordinated with metal ions in some complexes [13] and didn't participate in coordination in others compounds [14]. However, interestingly, although the ion SCN[−] didn't coordinate with metal ions in some complexes, the cell parameters of these complexes are different to those of the complex that obtained in the nonexistence of KSCN [10, 14]. In this paper, we reported a compound, [Hg(C₁₁H₁₁N₃)₂Cl₂], which was obtained in the mixed solution of HgCl₂, KSCN and bmi. Similarly to the reported compound [14], the ion SCN[−] didn't coordinate with metal ions, but it affected the crystal system and the space group of the compounds.

The titled compound is a mononuclear structure. As is shown in the upper part of the Fig., the Hg(II) atom is four-coordinated by two N atoms from two bmi ligands and two chlorido ligands. It crystallized in triclinic crystal system and space group $P\bar{1}$, differently to the reported compound that was obtained by the reaction of bmi and HgCl₂ [11], which is found to be monoclinic with space group *C2/c*. In the title compound, Hg–Cl bond lengths are 2.4297(12) and 2.4295(13) Å, respectively; and the Hg–N bond lengths are 2.311(4) and 2.224(4) Å, respectively. The bond angles around the Hg atom vary from 99.25(10)°

(N1–Hg1–Cl2) to $119.85(10)^\circ$ (N6–Hg1–Cl2). The dihedral angle between the imidazole planes in the two ligands is 79.6° , which is significantly different to that of the reported compound (47.3°) [12]. In the crystal, the adjacent complex molecules are stacked through the benzotriazol π – π interactions (the centroid–centroid distance is 3.543 and 3.896 Å, respectively) (lower part of the Figure) [17] and intermolecular interactions to form a supramolecular compound.

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