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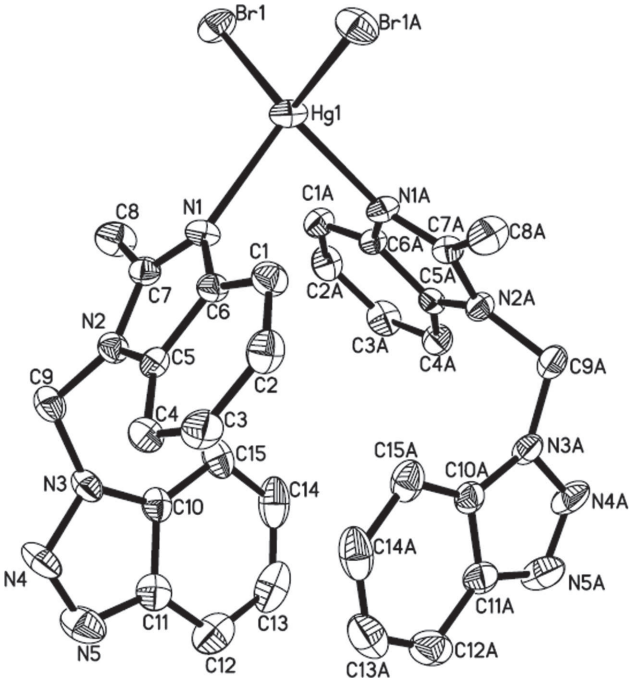
Crystal structure of dibromido-bis[μ-1-[(2-methyl-1*H*-benzoimidazol-1-yl)methyl]-1*H*-benzotriazole-κ*N*]mercury(II), $C_{30}H_{26}Br_2HgN_{10}$



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Abstract

$C_{30}H_{26}Br_2HgN_{10}$, monoclinic, *C*2/*c* (no. 15), $a = 15.5262(6)$ Å, $b = 13.2099(7)$ Å, $c = 14.8370(5)$ Å, $\beta = 95.688(3)°$, $V = 3028.1(2)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0329$, $wR_{ref}(F^2) = 0.0561$, $T = 291(2)$ K.

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

Table 1: Data collection and handling.

Crystal:	Colourless prism
	Size 0.24 × 0.20 × 0.18 mm
Wavelength:	Mo *Kα* radiation (0.71073 Å)
μ:	77.6 cm^{-1}
Diffractometer, scan mode:	Xcalibur, ω
$2\theta_{max}$, completeness:	52.8°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	6535, 3094, 0.030
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2484
$N(param)_{refined}$:	196
Programs:	SHELX [7], CrysAlis^{PRO} [8]

Source of material

The ligand 1-[(2-methyl-1*H*-benzoimidazol-1-yl)methyl]-1*H*-benzotriazole (0.04 mmol, 0.0105 g) in methanol (6 mL) was added dropwise to a methanol solution (6 mL) of $HgBr_2$ (0.04 mmol, 0.0144 g) in methanol. The resulting solution was allowed to stand at room temperature. After 2 weeks colourless crystals were obtained.

Experimental details

H atoms were generated geometrically and refined as riding atoms with C—H = 0.93 Å and U_{iso}(H) = 1.2 times U_{eq}(C) for aromatic H atoms, with C—H = 0.97 Å and U_{iso}(H) = 1.2 times, U_{eq}(C) for methylene H atoms, and with C—H = 0.96 Å and U_{iso}(H) = 1.5 times U_{eq}(C) for methyl H atoms.

Discussion

Imidazole and benzotriazole derivatives have been widely used in the syntheses of complexes since they can act as polydentate ligands and function as bridging ligands [1, 2]. Many symmetric imidazole and benzotriazole ligands have been applied [3, 4]. However, studies involving asymmetric imidazole and benzotriazole ligands are rather rare [5, 6].

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Hg1	0.5000	0.599472(19)	0.2500	0.04310(9)
Br1	0.36446(3)	0.70037(4)	0.19862(3)	0.05419(15)
N1	0.4768(2)	0.4742(2)	0.3552(2)	0.0370(8)
N2	0.4136(2)	0.3489(3)	0.4222(2)	0.0380(8)
N3	0.3603(2)	0.1793(3)	0.4198(2)	0.0432(9)
N4	0.3569(3)	0.1045(3)	0.4837(2)	0.0603(12)
N5	0.3669(3)	0.0177(3)	0.4452(3)	0.0709(13)
C1	0.6278(3)	0.4418(4)	0.4304(3)	0.0445(11)
H1	0.6548	0.4943	0.4025	0.053*
C2	0.6741(3)	0.3781(4)	0.4919(3)	0.0510(13)
H2	0.7334	0.3876	0.5051	0.061*
C3	0.6330(3)	0.3002(4)	0.5342(3)	0.0541(13)
H3	0.6658	0.2594	0.5757	0.065*
C4	0.5463(3)	0.2812(4)	0.5171(3)	0.0469(12)
H4	0.5194	0.2289	0.5455	0.056*
C5	0.5004(3)	0.3449(3)	0.4545(2)	0.0336(10)
C6	0.5397(3)	0.4242(3)	0.4121(2)	0.0344(10)
C7	0.4032(3)	0.4276(3)	0.3626(3)	0.0373(10)
C8	0.3178(3)	0.4549(4)	0.3160(3)	0.0588(13)
H8A	0.3209	0.5210	0.2896	0.088*
H8B	0.2754	0.4550	0.3589	0.088*
H8C	0.3017	0.4063	0.2692	0.088*
C9	0.3460(3)	0.2817(3)	0.4475(3)	0.0461(11)
H9A	0.3444	0.2838	0.5126	0.055*
H9B	0.2905	0.3049	0.4194	0.055*
C10	0.3718(3)	0.1377(4)	0.3378(3)	0.0426(11)
C11	0.3766(3)	0.0344(4)	0.3554(3)	0.0514(12)
C12	0.3886(3)	−0.0349(5)	0.2871(4)	0.0710(16)
H12	0.3915	−0.1041	0.2985	0.085*
C13	0.3960(3)	0.0027(6)	0.2030(4)	0.0768(18)
H13	0.4053	−0.0415	0.1561	0.092*
C14	0.3898(3)	0.1063(6)	0.1855(3)	0.0729(18)
H14	0.3940	0.1289	0.1267	0.088*
C15	0.3778(3)	0.1770(4)	0.2520(3)	0.0560(14)
H15	0.3740	0.2460	0.2400	0.067*

We are engaged in the synthesis of unsymmetrical *N*-heterocyclic ligands and synthesized compound 1-[(2-methyl-1*H*-benzoimidazol-1-yl)methyl]-1*H*-benzotriazole. As part of this study, we selected this compound as ligand and generate a new complex $[Hg(C_{15}H_{13}N_5)_2Br_2]$, which is reported here.

The title compound is a mononuclear complex, located on a two-fold axis in the space group *C*2/*c*. As is shown in the figure, the Hg(II) atom is four-coordinated by two N atoms from two 1-[(2-methyl-1*H*-benzoimidazol-1-yl)methyl]-1*H*-benzotriazole ligands and two Br atoms in a distorted tetrahedral coordination environment (with Hg—N bond length of 2.327(3) Å, with Hg—Br bond length of 2.5433(5) Å). The bond angles around Hg(II) ion range from 89.35 to 116.79°. In addition, the benzoimidazol rings in adjacent molecules are almost parallel. The average interplanar distance is 3.54 Å, which suggests π−π interactions.

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