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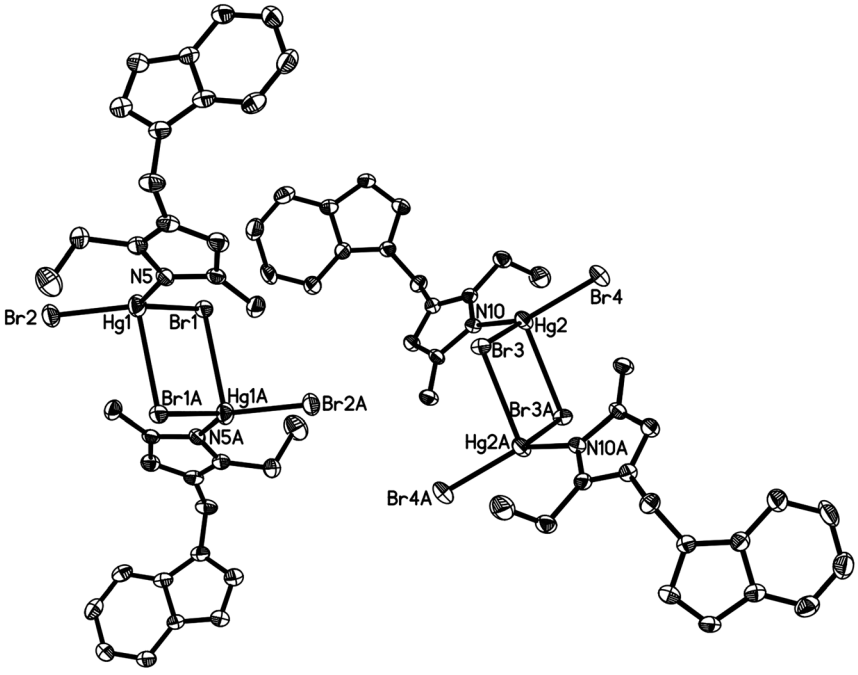
Crystal structure of the dinuclear mercury(II) complex bis(μ^2-bromido)-dibromido-bis{1-[(benzotriazol-1-yl)methyl]-1-*H*-1,3-(2-ethyl-5-methyl-imidazol)-κ^1*N*} dimercury(II), $C_{26}H_{30}N_{10}Hg_2Br_4$



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Abstract

$C_{26}H_{30}N_{10}Hg_2Br_4$, triclinic, $P\bar{1}$ (no. 2), a = 8.8582(4) Å, b = 11.5968(5) Å, c = 17.4657(10) Å, α = 107.564(5)°, β = 92.283(4)°, γ = 97.388(4)°, V = 1690.47(15) Å^3, Z = 2, $R_{gt}(F)$ = 0.0423, $\omega R_{ref}(F^2)$ = 0.1112, T = 293 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.

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.20 × 0.12 × 0.11 mm
Wavelength:	Cu *K*α radiation (1.54184 Å)
μ:	21.9 mm^{-1}
Diffractometer, scan mode:	Xcalibur, ω
θ_{max}, completeness:	67.1°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	12,068, 6,038, 0.042
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 4,982
$N(param)_{refined}$:	384
Programs:	CrysAlis^{PRO},[1] Olex2,[2] SHELX[3]

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

Atom	*X*	*y*	*z*	U_{iso}*/U_{eq}
Hg1	0.45121 (4)	0.99516 (4)	0.61095 (2)	0.05519 (14)
Br1	0.56215 (10)	0.83714 (8)	0.49456 (6)	0.0451 (2)
Br2	0.63512 (13)	1.13500 (9)	0.72068 (7)	0.0621 (3)
N1	−0.0465 (10)	0.6891 (7)	0.8102 (5)	0.0552 (19)
N2	−0.0286 (10)	0.7967 (8)	0.8027 (5)	0.056 (2)
N3	−0.1255 (8)	0.7969 (7)	0.7401 (5)	0.0454 (16)
N4	−0.0148 (8)	0.9161 (7)	0.6595 (5)	0.0465 (17)
N5	0.2006 (8)	0.9559 (6)	0.6106 (4)	0.0408 (15)
C1	−0.3175 (11)	0.6347 (9)	0.6418 (6)	0.053 (2)
H1	−0.3503	0.6815	0.6114	0.064*
C2	−0.3764 (12)	0.5156 (11)	0.6261 (6)	0.061 (3)
H2	−0.4522	0.4803	0.5841	0.074*
C3	−0.3266 (12)	0.4426 (9)	0.6716 (6)	0.058 (2)
H3	−0.3691	0.3608	0.6587	0.070*
C4	−0.2163 (11)	0.4920 (9)	0.7344 (6)	0.054 (2)
H4	−0.1838	0.4454	0.7651	0.065*
C5	−0.1547 (11)	0.6141 (8)	0.7506 (5)	0.046 (2)
C6	−0.2067 (9)	0.6831 (8)	0.7050 (5)	0.0434 (19)
C7	−0.1274 (11)	0.9072 (8)	0.7168 (6)	0.053 (2)
H7A	−0.1060	0.9784	0.7644	0.063*
H7B	−0.2284	0.9065	0.6928	0.063*
C8	−0.0382 (10)	0.8631 (8)	0.5778 (6)	0.049 (2)
H8	−0.1290	0.8188	0.5494	0.059*
C9	0.0965 (10)	0.8872 (7)	0.5453 (5)	0.0422 (18)
C10	0.1295 (10)	0.9711 (8)	0.6772 (5)	0.0453 (19)
C11	0.1342 (11)	0.8557 (10)	0.4612 (6)	0.057 (2)
H11A	0.1985	0.9236	0.4532	0.086*
H11B	0.0420	0.8370	0.4263	0.086*
H11C	0.1870	0.7858	0.4491	0.086*
C12	0.1988 (13)	1.0464 (9)	0.7597 (6)	0.056 (2)
H12A	0.3041	1.0337	0.7659	0.067*
H12B	0.1437	1.0203	0.7999	0.067*
C13	0.1931 (18)	1.1827 (11)	0.7735 (9)	0.095 (4)
H13A	0.2415	1.2073	0.7316	0.142*
H13B	0.2455	1.2295	0.8248	0.142*
H13C	0.0886	1.1966	0.7728	0.142*
Hg2	0.05463 (4)	0.34800 (3)	0.02593 (2)	0.04688 (13)
Br3	−0.06479 (9)	0.54150 (8)	0.10582 (5)	0.0408 (2)
Br4	−0.11274 (15)	0.15346 (10)	−0.04530 (8)	0.0708 (3)
N6	0.5927 (10)	0.1963 (7)	0.3097 (5)	0.055 (2)
N7	0.5717 (9)	0.1798 (7)	0.2324 (5)	0.0516 (18)
N8	0.6399 (8)	0.2795 (6)	0.2159 (4)	0.0412 (15)
N9	0.5161 (7)	0.3448 (6)	0.1138 (4)	0.0366 (14)
N10	0.2989 (7)	0.3770 (6)	0.0655 (4)	0.0342 (13)
C14	0.7333 (12)	0.3675 (10)	0.4252 (6)	0.060 (3)
H14	0.7138	0.3310	0.4652	0.071*
C15	0.8161 (13)	0.4820 (12)	0.4418 (7)	0.070 (3)
H15	0.8528	0.5249	0.4948	0.083*
C16	0.8472 (14)	0.5363 (11)	0.3808 (7)	0.076 (4)
H16	0.9040	0.6140	0.3948	0.091*
C17	0.7962 (12)	0.4783 (10)	0.3019 (6)	0.062 (3)
H17	0.8180	0.5138	0.2617	0.075*
C18	0.7098 (10)	0.3628 (8)	0.2849 (5)	0.0422 (18)
C19	0.6804 (10)	0.3095 (8)	0.3449 (6)	0.0454 (19)
C20	0.6382 (9)	0.2833 (8)	0.1349 (5)	0.0423 (18)
H20A	0.6262	0.2003	0.0985	0.051*
H20B	0.7357	0.3253	0.1274	0.051*
C21	0.5314 (9)	0.4682 (7)	0.1225 (5)	0.0393 (17)
H21	0.6169	0.5261	0.1450	0.047*
C22	0.3974 (9)	0.4888 (7)	0.0919 (5)	0.0366 (16)
C23	0.3732 (9)	0.2920 (7)	0.0785 (5)	0.0368 (16)
C24	0.3554 (10)	0.6064 (7)	0.0859 (6)	0.0450 (19)
H24A	0.3151	0.5950	0.0319	0.067*
H24B	0.4444	0.6676	0.0994	0.067*
H24C	0.2795	0.6323	0.1226	0.067*
C25	0.3170 (10)	0.1589 (8)	0.0544 (6)	0.048 (2)
H25A	0.2081	0.1463	0.0600	0.058*
H25B	0.3674	0.1230	0.0900	0.058*
C26	0.3473 (18)	0.0950 (10)	−0.0323 (7)	0.084 (4)
H26A	0.2969	0.1299	−0.0678	0.126*
H26B	0.3088	0.0094	−0.0463	0.126*
H26C	0.4552	0.1054	−0.0376	0.126*

1 Source of material

A methanol solution (4 mL) of KSCN (0.05 mmol) was added dropwise into a methanol solution (2 mL) of $HgBr_2$ (0.05 mmol), giving a clear solution. 1-[(benzotriazol-1-yl) methyl]-1-*H*-1,3-(2-ethyl-5-methyl-imidazol) (0.05 mmol) in 4 mL of methanol was added dropwise to the above mixture solution. The resulting solution was left at room temperature. After four days, colorless crystals were obtained.

2 Experimental details

H atoms were generated geometrically, with C–H = 0.96, 0.97 and 0.93 Å for methyl, methylene and aromatic H, respectively, and constrained to ride on their parent atoms with U_{iso}(H) = *x* times U_{eq}(C), where *x* = 1.5 for methyl H and *x* = 1.2 for all other H atoms.

3 Comment

For the past few decades, the rational design coordination compounds have received remarkable attention, owing to their fascinating structural versatility and special functionality in photoluminescence, catalysis, magnetics, and so on.[4,5] Multidentate N-heterocyclic compounds are often employed as ligands to produce coordination compounds due to their rich coordination sites and various coordination

modes. A large number of appealing complexes based on these ligands have been reported.[6,7] For some time now our group has been dedicated to the synthesis of N-heterocyclic compounds and the coordination performance studies.[8–10] We synthesized some compounds based on the imidazole and benzotriazole, such as 1-[(benzotriazol-1-yl)methyl]-1-*H*-1,3-(2-methyl-imidazol), 1-[(benzotriazol-1-yl)methyl]-1-*H*-1,3-(2-ethyl-imidazol) and 1-[(benzotriazol-1-yl)methyl]-1-*H*-1,3-(2-isopropyl-imdazol), and studied their coordination behavior with transitional metal ions in different environments, obtaining a series of CPs.[11–18] As a continuation of our research, recently, we have prepared a compound 1-[(benzotriazol-1-yl)methyl]-1-*H*-1,3-(2-ethyl-5-methyl-imidazol) (bmemi) and used it as ligand to react with $HgBr_2$ in the presence of KSCN, generating a new coordination compound, which is reported here.

Crystal structure analysis reveals that the title compound is a dinuclear complex. As is shown in the figure, all mercury ions are in a distorted coordination tetrahedral environment where each of them is surrounded by one N atom from a bmemi ligand and three (two bridge and one terminal) Br atoms. There are slight differences in bond lengths and bond angles around Hg1 and Hg2 ions. The bond length of Hg1–N5 is 2.207 (7) Å, and the bond length of Hg2–N10 is 2.197 (6) Å. Hg1–Br bond lengths are between 2.4805(11) and 3.0655(10) Å, and Hg2–Br bond lengths fall in the range of 2.4768(11)–2.9517(9) Å. The bond angles around the Hg1 atom vary from 89.79(3)° (Br1–Hg1–Br1A) to 128.02(19)° (N5–Hg1–Br2), and the bond angles around the Hg2 atom are within the range of 85.32(3) (Br3–Hg2–Br3A)–128.53(17)° (N10–Hg2–Br4). The distance of Hg1–Hg1A is 4.036 Å, and that of Hg2–Hg2A is 4.113 Å.

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