Crystal structure of bis{1-[(benzotriazol-1-yl)methyl]-1-*H*-1,3-(2-methyl-imdazol)}dibromidomercury(II), [Hg(C₁₁H₁₁N₅)₂Br₂], C₂₂H₂₂Br₂HgN₁₀

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Abstract

C₂₂H₂₂Br₂HgN₁₀, monoclinic, *P*₂₁/*c* (no. 14), *a* = 7.2071(3) Å, *b* = 27.4869(12) Å, *c* = 13.3612(4) Å, β = 103.638(3)°, *V* = 2572.3 Å³, *Z* = 4, *R*_{gt}(*F*) = 0.0383, *wR*_{ref}(*F*²) = 0.0788, *T* = 291 K.

Table 1. Data collection and handling.

Crystal:	colourless blocks, size 0.16×0.18×0.2 mm
Wavelength:	Mo <i>K</i> _α radiation (0.7107 Å)
μ:	91.22 cm ^{−1}
Diffractometer, scan mode:	Xcalibur, Eos, Gemini, ω
2θ _{max} :	52.74°
<i>N</i> (<i>hkl</i>) _{measured} , <i>N</i> (<i>hkl</i>) _{unique} :	20189, 5236
Criterion for <i>I</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} :	<i>I</i> _{obs} > 2 σ(<i>I</i> _{obs}), 4218
<i>N</i> (<i>param</i>) _{refined} :	318
Programs:	SHELX [12], CrysAlisPRO [13], OLEX2 [14]

Source of material

A methanol solution (5 mL) of 1-[(benzotriazol-1-yl)methyl]-1-*H*-1,3-(2-methyl-imdazol) (0.1 mmol) was added dropwise into a methanol solution (3 mL) of HgBr₂ (0.05 mmol). The resulting solution was left at room temperature. After three days, quality, colourless crystals were obtained from the solution.

Discussion

Polymeric coordination compounds have attracted interest because of their interesting structures, topologies, properties and their potential applications as functional materials [1, 2]. Multidentate *N*-hetero-cyclic ligands containing rich coordination sites, such as imidazole, triazole, tetrazole and their derivative are often employed to produce polymeric networks with structural diversity owing to their various coordination modes. Plenty of appealing coordination frameworks based on these ligands has been reported [3–6]. For some time now we have involved in the synthesis of a series of multidentate *N*-heterocyclic compounds and studied their coordination behaviors [7–11]. In this paper, we use a *N*-heterocyclic compound, 1-[(benzotriazol-1-yl)methyl]-1-*H*-1,3-(2-methyl-imdazol), as ligand to react with HgBr₂, generating a new coordination compound, [Hg(C₁₁H₁₁N₅)₂Br₂], which is reported here. In the

title complex, [Hg(C₁₁H₁₁N₅)₂Br₂], the Hg atom has a distorted tetrahedral coordination formed by the two imidazole N atoms of two 1-[(benzotriazol-1-yl)methyl]-1-*H*-1,3-(2-methyl-imdazol) ligands and two terminal bromido ligands (Fig.). The bond lengths of Hg–N are 2.292(4), 2.338(4) Å, whereas those of Hg–Br are 2.5017(6), and 2.5283(6) Å. The bond angles around the Hg atom vary from 93.63(15)° (N1–Hg1–N6) to 125.44(2)° (Br2–Hg1–Br1). The dihedral angle between the imidazole planes in the two ligands is 70.4(2)°.

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(1)	4e	1.1483	0.525	0.9554	0.051
H(2)	4e	0.8664	0.5766	0.9274	0.056
H(4A)	4e	1.0466	0.5261	0.5967	0.071
H(4B)	4e	0.8583	0.5568	0.5784	0.071
H(4C)	4e	0.8514	0.5003	0.5938	0.071
H(5A)	4e	0.5914	0.5668	0.6689	0.062
H(5B)	4e	0.5895	0.5942	0.7714	0.062
H(8)	4e	0.7410	0.7793	0.5868	0.070
H(9)	4e	0.8243	0.8095	0.7513	0.079
H(10)	4e	0.8682	0.7586	0.8919	0.079
H(11)	4e	0.8086	0.6756	0.8731	0.063
H(12)	4e	1.0715	0.3847	0.5599	0.054
H(13)	4e	0.7944	0.3316	0.5418	0.055
H(15A)	4e	0.8963	0.3755	0.8959	0.082
H(15B)	4e	0.7575	0.4175	0.8464	0.082
H(15C)	4e	0.9780	0.4271	0.8799	0.082
H(16A)	4e	0.5621	0.3518	0.7524	0.049
H(16B)	4e	0.5275	0.3247	0.6464	0.049
H(19)	4e	0.8061	0.1409	0.8526	0.056
H(20)	4e	0.7554	0.1108	0.6867	0.063
H(21)	4e	0.6692	0.1615	0.5470	0.061
H(22)	4e	0.6246	0.2436	0.5643	0.051

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Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Hg(1)	4e	1.28905(3)	0.454752(8)	0.77437(2)	0.0399(1)	0.0377(2)	0.0487(1)	0.0048(1)	0.01191(9)	0.0062(1)
Br(1)	4e	1.4261(1)	0.42078(3)	0.95230(5)	0.0550(4)	0.1383(8)	0.0597(4)	0.0402(5)	0.0195(3)	0.0454(4)
Br(2)	4e	1.46919(9)	0.46631(2)	0.63736(5)	0.0572(4)	0.0644(4)	0.0539(3)	−0.0085(3)	0.0238(3)	0.0018(3)
N(1)	4e	1.0947(6)	0.5178(2)	0.7971(3)	0.044(3)	0.028(3)	0.032(2)	0.005(2)	0.008(2)	0.003(2)
N(2)	4e	0.8408(6)	0.5636(2)	0.7723(3)	0.040(3)	0.031(2)	0.043(2)	0.009(2)	0.011(2)	0.002(2)
N(3)	4e	0.6946(6)	0.6337(2)	0.6739(3)	0.042(3)	0.032(3)	0.051(3)	0.008(2)	0.001(2)	−0.005(2)
N(4)	4e	0.6483(8)	0.6367(2)	0.5703(4)	0.083(4)	0.054(4)	0.051(3)	0.020(3)	−0.010(3)	−0.014(3)
N(5)	4e	0.6646(9)	0.6818(2)	0.5442(4)	0.099(5)	0.053(4)	0.048(3)	0.016(3)	−0.008(3)	−0.002(3)
N(6)	4e	1.0336(6)	0.4034(1)	0.7027(3)	0.047(3)	0.028(2)	0.037(2)	−0.006(2)	0.014(2)	0.000(2)
N(7)	4e	0.7826(6)	0.3571(2)	0.6861(3)	0.038(2)	0.030(2)	0.031(2)	−0.004(2)	0.005(2)	0.002(2)
N(8)	4e	0.6777(6)	0.2862(2)	0.7627(3)	0.038(3)	0.033(3)	0.031(2)	−0.006(2)	0.007(2)	0.001(2)
N(9)	4e	0.7249(7)	0.2838(2)	0.8670(3)	0.055(3)	0.052(3)	0.031(2)	−0.006(3)	0.014(2)	−0.005(2)
N(10)	4e	0.7661(7)	0.2391(2)	0.8950(3)	0.062(3)	0.048(3)	0.031(2)	−0.001(3)	0.011(2)	0.004(2)
C(1)	4e	1.0699(9)	0.5331(2)	0.8918(4)	0.059(4)	0.037(3)	0.029(3)	0.001(3)	0.006(2)	0.003(2)
C(2)	4e	0.9148(9)	0.5614(2)	0.8768(4)	0.068(4)	0.040(3)	0.036(3)	0.006(3)	0.022(3)	−0.004(2)
C(3)	4e	0.9550(8)	0.5365(2)	0.7262(4)	0.039(3)	0.026(3)	0.034(3)	0.004(2)	0.009(2)	0.002(2)
C(4)	4e	0.9252(9)	0.5293(2)	0.6139(4)	0.056(4)	0.050(4)	0.033(3)	0.009(3)	0.004(2)	−0.002(2)
C(5)	4e	0.6647(8)	0.5882(2)	0.7213(5)	0.036(3)	0.039(4)	0.075(4)	0.011(3)	0.004(3)	−0.008(3)
C(6)	4e	0.7401(7)	0.6785(2)	0.7163(4)	0.027(3)	0.037(3)	0.054(3)	0.008(3)	0.009(2)	−0.004(3)
C(7)	4e	0.7222(8)	0.7089(2)	0.6320(4)	0.045(4)	0.042(4)	0.056(4)	0.012(3)	0.006(3)	−0.001(3)
C(8)	4e	0.7540(9)	0.7589(2)	0.6435(5)	0.052(4)	0.047(4)	0.073(4)	0.005(3)	0.011(3)	0.005(3)
C(9)	4e	0.8047(9)	0.7762(3)	0.7409(6)	0.051(4)	0.044(4)	0.100(6)	−0.007(3)	0.017(4)	−0.009(4)
C(10)	4e	0.8285(9)	0.7454(3)	0.8262(5)	0.055(4)	0.069(5)	0.073(5)	−0.006(4)	0.011(3)	−0.034(4)
C(11)	4e	0.7950(9)	0.6959(2)	0.8162(4)	0.054(4)	0.057(4)	0.045(3)	0.010(3)	0.009(3)	−0.005(3)
C(12)	4e	0.9995(9)	0.3806(2)	0.6086(4)	0.070(4)	0.036(3)	0.032(3)	−0.002(3)	0.020(3)	0.004(2)
C(13)	4e	0.8464(9)	0.3515(2)	0.5977(4)	0.070(4)	0.035(3)	0.031(3)	−0.006(3)	0.011(3)	0.002(2)
C(14)	4e	0.9007(7)	0.3888(2)	0.7487(3)	0.036(3)	0.025(3)	0.033(3)	0.001(2)	0.008(2)	−0.002(2)
C(15)	4e	0.8815(9)	0.4035(2)	0.8517(4)	0.054(4)	0.064(4)	0.053(3)	−0.017(3)	0.027(3)	−0.021(3)
C(16)	4e	0.6215(8)	0.3313(2)	0.7099(4)	0.038(3)	0.038(3)	0.044(3)	0.001(3)	0.007(2)	−0.001(2)
C(17)	4e	0.6908(7)	0.2411(2)	0.7222(3)	0.027(3)	0.031(3)	0.037(3)	−0.007(2)	0.010(2)	−0.001(2)
C(18)	4e	0.7475(7)	0.2108(2)	0.8080(4)	0.038(3)	0.039(3)	0.036(3)	−0.009(3)	0.014(2)	0.006(2)
C(19)	4e	0.7710(8)	0.1614(2)	0.7960(4)	0.050(4)	0.037(4)	0.056(4)	−0.003(3)	0.019(3)	0.010(3)
C(20)	4e	0.7404(8)	0.1439(2)	0.6973(5)	0.054(4)	0.037(4)	0.075(4)	−0.003(3)	0.031(3)	−0.004(3)
C(21)	4e	0.6873(9)	0.1748(2)	0.6126(4)	0.060(4)	0.048(4)	0.048(3)	−0.014(3)	0.022(3)	−0.014(3)
C(22)	4e	0.6606(8)	0.2234(2)	0.6214(4)	0.055(4)	0.040(4)	0.034(3)	−0.014(3)	0.010(2)	−0.004(2)

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