Crystal structure of tetraiodobis[μ-(1,1′-(1,5-pentanediyl)-bis-1*H*-benzimidazole)]dimercury(II), $[HgI_2(C_{19}H_{20}N_4)]_2$

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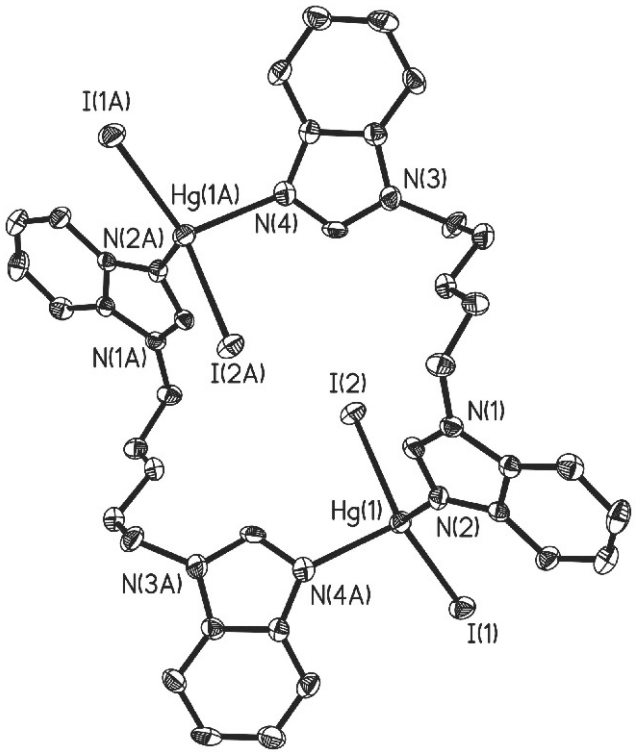

Abstract

$C_{19}H_{20}HgI_2N_4$, monoclinic, *C*12/*c*1 (no. 15), a = 19.471(2) Å, b = 10.564(1) Å, c = 21.295(3) Å, β = 100.34(1)°, V = 4309.1 Å^3, Z = 8, $R_{gt}(F)$ = 0.041, $wR_{ref}(F^2)$ = 0.087, T = 296 K.

Source of material

A methanol solution (6 ml) of 1,1′-(1,5-pentanediyl)bis-1*H*-benzimidazole (pbbm, 30.4 mg, 0.1 mmol) was laid carefully above a DMF solution (4 ml) of HgI_2 (45.4 mg, 0.1 mmol). Colorless crystals suitable for X-ray diffraction were obtained three days later.

Elemental analysis — found: C, 30.11 %, H, 2.63 %, N, 7.41 %; calculated for $C_{19}H_{20}HgI_2N_4$: C, 30.07 %, H, 2.66 %, N, 7.38 %.

Experimental details

All the hydrogen atoms were included in calculated positions and treated as riding with d(O—H) = 0.85 Å, d(C—H) = 0.93 Å and U_{iso}(H) = 1.2 U_{eq}(C,O).

Discussion

In the search for supramolecular coordination networks with intriguing architectures and topologies, a marked increase in both interest and research activity has been given to extended solids of metals with d^{10} configuration involving mercury because of their various coordination configurations and coordination numbers [1-3]. Especially some mercury(II) iodide complexes often behave differently compared with the chloride and bromide complexes. Such as in the series $HgX_2(pyridine)_2$, the chloro derivative possesses an octahedral, halide-bridged polymeric structure, but the bromo and iodo derivatives are monomeric [4,5]. In these complexes, the mercury typically has a lower coordination number of four. It has been suggested that this tendency of iodine to lower the coordination number of the d^{10} metal atom is due to an increase in electron density at the metal center caused by the softer character of iodine relative to the lighter halogens, and may also be related to the larger size of iodine [6].

The asymmetric unit of the title crystal structure consists of a HgI_2 molecule and half of a 1,1′-(1,5-pentanediyl)bis-1*H*-benzimidazole (pbbm) ligand binding to Hg^{2+} atom. The Hg^{2+} atom is coordinated by two pbbm ligands and two iodide ions in a distorted tetrahedral manner. The distortion is probably the result of the strong preference of Hg^{2+} for the soft donor iodine atoms. The bond lengths d(Hg—I1), d(Hg—I2), and d(Hg—N) are 2.6513(7), 2.7156(7), 2.302(6) and 2.418(7) Å, respectively, which are similar to those of the related complexes $[HgI_2(L)]_n$ (d(Hg—I) ranging from 2.6430(5) to 2.6683(8) Å, and d(Hg—N) from 2.3626(6) to 2.457(6) Å) [7-9]. Larger I–Hg–I angles (131.12 (2) °) and smaller N–Hg–N angles (92.7 (2) °) in the complex are consistent with the preference of $Hg^{2+}$for I^-.

Table 1. Data collection and handling.

Crystal:	colorless block, size 0.11 × 0.15 × 0.23 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	100.20 cm^{-1}
Diffractometer, scan mode:	Xcalibur Eos Gemini, φ/ω
$2\theta_{max}$:	51°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	8677, 4007
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 3195
$N(param)_{refined}$:	235
Programs:	SHELXS-97, SHELXL-97, SHELXTL [10]

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

Atom	Site	x	y	z	U_{iso}
H(1)	8*f*	0.3688	0.6530	0.5156	0.041
H(3)	8*f*	0.5889	0.5014	0.6316	0.053
H(4)	8*f*	0.6906	0.5785	0.6032	0.062
H(5)	8*f*	0.6877	0.7266	0.5258	0.058
H(6)	8*f*	0.5847	0.8010	0.4673	0.051
H(8A)	8*f*	0.4622	0.4298	0.6245	0.053
H(8B)	8*f*	0.3852	0.4720	0.5978	0.053
H(9A)	8*f*	0.4211	0.5216	0.7082	0.056
H(9B)	8*f*	0.4768	0.6145	0.6896	0.056
H(10A)	8*f*	0.3326	0.6454	0.6597	0.056
H(10B)	8*f*	0.3840	0.7315	0.6304	0.056
H(11A)	8*f*	0.3751	0.7251	0.7609	0.065
H(11B)	8*f*	0.4304	0.8064	0.7339	0.065
H(12A)	8*f*	0.3412	0.9374	0.7497	0.064
H(12B)	8*f*	0.3407	0.9294	0.6762	0.064
H(13)	8*f*	0.2350	0.8080	0.6082	0.048
H(15)	8*f*	0.0694	0.6754	0.7329	0.056
H(16)	8*f*	0.0932	0.6983	0.8421	0.066
H(17)	8*f*	0.1947	0.7892	0.8930	0.067
H(18)	8*f*	0.2794	0.8603	0.8350	0.060

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)	8*f*	0.40227(2)	0.88864(3)	0.42880(2)	0.0351(2)	0.0441(2)	0.0390(2)	–0.0017(1)	0.0093(2)	0.0045(2)
I(1)	8*f*	0.48761(3)	1.03326(5)	0.37602(3)	0.0563(4)	0.0462(3)	0.0519(4)	–0.0135(3)	0.0219(3)	–0.0009(3)
I(2)	8*f*	0.29444(3)	0.94926(5)	0.48825(3)	0.0397(3)	0.0490(4)	0.0580(4)	–0.0007(3)	0.0217(3)	–0.0008(3)
N(1)	8*f*	0.4564(3)	0.5785(5)	0.5662(3)	0.039(4)	0.034(3)	0.031(4)	–0.002(3)	0.010(3)	–0.004(3)
N(2)	8*f*	0.4535(3)	0.7213(6)	0.4889(3)	0.032(4)	0.039(4)	0.039(5)	–0.007(3)	0.004(3)	–0.001(3)
N(3)	8*f*	0.2592(4)	0.8403(6)	0.7024(4)	0.041(4)	0.040(4)	0.046(5)	–0.008(3)	0.007(4)	–0.009(3)
N(4)	8*f*	0.1599(3)	0.7494(6)	0.6527(3)	0.040(4)	0.038(4)	0.041(5)	–0.001(3)	0.003(3)	0.000(3)
C(1)	8*f*	0.4173(4)	0.6518(7)	0.5220(4)	0.034(4)	0.040(4)	0.027(5)	0.002(4)	0.001(4)	0.001(4)
C(2)	8*f*	0.5254(4)	0.6047(6)	0.5639(4)	0.038(5)	0.026(4)	0.032(5)	–0.005(3)	0.006(4)	–0.004(3)
C(3)	8*f*	0.5877(4)	0.5599(8)	0.5988(4)	0.049(6)	0.044(5)	0.039(6)	0.008(4)	0.004(4)	0.008(4)
C(4)	8*f*	0.6476(4)	0.6073(8)	0.5819(5)	0.029(5)	0.042(5)	0.082(8)	0.005(4)	0.003(5)	–0.006(5)
C(5)	8*f*	0.6456(4)	0.6958(8)	0.5345(5)	0.032(5)	0.047(5)	0.066(7)	–0.005(4)	0.011(5)	0.001(5)
C(6)	8*f*	0.5848(4)	0.7411(7)	0.4994(4)	0.039(5)	0.043(5)	0.047(6)	–0.009(4)	0.014(4)	–0.001(4)
C(7)	8*f*	0.5228(4)	0.6923(6)	0.5142(4)	0.033(4)	0.026(4)	0.028(5)	0.001(3)	0.006(4)	–0.010(3)
C(8)	8*f*	0.4319(5)	0.5026(7)	0.6145(4)	0.055(6)	0.041(5)	0.037(6)	–0.001(4)	0.012(4)	0.010(4)
C(9)	8*f*	0.4308(5)	0.5787(8)	0.6752(4)	0.051(6)	0.054(5)	0.035(6)	–0.009(4)	0.010(4)	0.014(4)
C(10)	8*f*	0.3789(4)	0.6826(8)	0.6678(4)	0.038(5)	0.061(6)	0.040(6)	–0.011(4)	0.004(4)	–0.011(4)
C(11)	8*f*	0.3834(4)	0.7726(9)	0.7240(5)	0.042(5)	0.071(6)	0.050(7)	–0.016(5)	0.009(5)	–0.018(5)
C(12)	8*f*	0.3326(4)	0.8815(8)	0.7130(5)	0.042(5)	0.052(6)	0.071(8)	–0.019(5)	0.024(5)	–0.017(5)
C(13)	8*f*	0.2203(4)	0.8003(7)	0.6472(4)	0.053(6)	0.043(5)	0.027(5)	–0.005(4)	0.019(4)	–0.003(4)
C(14)	8*f*	0.1600(4)	0.7547(6)	0.7180(4)	0.037(5)	0.022(4)	0.042(6)	–0.001(3)	0.005(4)	–0.005(3)
C(15)	8*f*	0.1110(4)	0.7123(7)	0.7530(5)	0.039(5)	0.043(5)	0.059(7)	–0.010(4)	0.015(5)	–0.002(4)
C(16)	8*f*	0.1256(5)	0.7264(9)	0.8180(5)	0.061(7)	0.063(6)	0.042(7)	0.003(5)	0.015(5)	–0.006(5)
C(17)	8*f*	0.1869(5)	0.7809(8)	0.8489(5)	0.070(7)	0.064(6)	0.041(6)	0.010(5)	0.027(5)	–0.014(5)
C(18)	8*f*	0.2377(5)	0.8241(8)	0.8149(4)	0.044(5)	0.065(6)	0.040(6)	0.010(5)	0.001(4)	–0.018(5)
C(19)	8*f*	0.2213(4)	0.8090(7)	0.7492(4)	0.042(5)	0.037(5)	0.039(6)	0.004(4)	0.008(4)	–0.008(4)

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