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Two new isostructural mercury(II) complexes involving the N-heterocyclic 1-[(benzotriazol-1-yl)methyl]-1*H*-1,3-imidazole ligand: syntheses, structures and properties

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Two new isostructural mercury(II) complexes involving N-heterocyclic ligand 1-((benzotriazol-1-yl)methyl)-1*H*-1,3-imidazole: syntheses, structures, and properties

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Table S1. Selected crystal structure data for complexes (I), (II) and the related complexes.

complex	space group	<i>a</i> , Å	<i>b</i> , Å	<i>c</i> , Å	<i>α</i> , deg	<i>β</i> , deg	<i>γ</i> , deg	Ref.
[Hg(bmi)Cl ₂] ₂	<i>P</i> -1	7.6448(15)	9.5454(19)	9.5761(19)	81.41(3)	86.20(3)	71.15(3)	[1]
[Hg(bmi) ₂ Br ₂](I)	<i>Pbcn</i>	11.756(2)	11.764(2)	17.407(4)	90	90	90	This work
[Hg(bmi) ₂ I ₂](II)	<i>Pbcn</i>	12.103(2)	11.827(2)	17.862(4)	90	90	90	This work
[Hg(bimt)Br ₂] ₂ ·H ₂ O	<i>P</i> 2 ₁ / <i>n</i>	7.4937(15)	20.899(4)	9.1612(18)	90	104.81(3)	90	[2]
[Hg(bimt)I ₂] ₂	<i>C</i> 2/ <i>c</i>	22.096(4)	7.4490(15)	16.889(3)	90	90.77(3)	90	[2]
[Hg(imb) ₂ I ₂]	<i>P</i> 2 ₁ / <i>c</i>	14.817(3)	18.370(4)	9.724(2)	90	103.11(3)	90	[3]

bimt = 1-[(1*H*-benzimidazol-2-yl)methyl]-1*H*-tetrazole, imb = 2-(1*H*-imidazole-1-ylmethyl)-1*H*-benzimidazole

[1] Duan, L. K., Liu, S. L., Zhou, W. & Meng, X. R. (2010). *Synth. React. Inorg. Met.-Org. Chem.* **40**, 319-327.

[2] Ding, Y. N., Zhou, X. L., Jin, G. H., Zhao, D. & Meng, X. R. (2012). *Synth. React. Inorg. Met.-Org. Chem.* **42**, 438-443.

[3] Yan, S. X., Jin, G. H., Yang, Y., Su, X. & Meng, X. R. (2012). *Synth. React. Inorg. Met.-Org. Chem.* **42**, 678-684.

Table S2. Selected bond lengths (Å) and angles (°) of complexes (I) and (II)

Complex (I)		Complex (II)	
Hg1—N1	2.304 (4)	Hg1—N1	2.340 (5)
Hg1—Br1	2.5226 (8)	Hg1—I1	2.6659 (6)
N1—Hg1—N1i	106.9 (2)	N1—Hg1—N1i	104.0 (3)

N1—Hg1—Br1	109.41 (13)	N1—Hg1—I1	108.14 (15)
N1—Hg1—Br1i	101.61 (13)	N1—Hg1—I1i	101.36 (15)
Br1i—Hg1—Br1	126.78 (4)	I1i—Hg1—I1	131.23 (3)