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Crystal structure of *catena*-poly[(μ_2 -1-((benzotriazol-1-yl)methyl)-1*H*-1,3-imdazole- κ^2 *N:N'*)-(1-((benzotriazol-1-yl)methyl)-1*H*-1,3-imdazole- κ^1 *N*)-(methanol- κ^1 *O*)mercury(II)] dinitrate, $C_{21}H_{22}N_{12}O_7Hg$

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Abstract

$C_{21}H_{22}N_{12}O_7Hg$, monoclinic, $P2_1/n$ (no. 13), $a = 13.655(3)$ Å, $b = 8.7038(17)$ Å, $c = 23.260(5)$ Å, $\beta = 102.51(3)^\circ$, $V = 2698.8(10)$ Å³, $Z = 4$, $R_{gt}(F) = 0.0446$, $wR_{ref}(F^2) = 0.0875$, $T = 293(2)$ 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.

Source of material

All chemicals were of reagent grade quality obtained from commercial sources and used without further purification. A methanol solution (3 mL) of bmi (0.1 mmol) is added dropwise into an aqueous solution (2 mL) of $Hg(NO_3)_2$ (0.1 mmol) to give a clear solution. The resultant solution was allowed to stand at room temperature. Good quality colourless crystals were obtained after 3 weeks (yield 39%, based on Hg).

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Table 1: Data collection and handling.

Crystal:	Colourless platelike
Size:	$0.12 \times 0.10 \times 0.06$ mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	5.77 mm ⁻¹
Diffractometer, scan mode:	Rigaku Saturn, ω
θ_{max} , completeness:	25.5° , 99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int} :	12128, 5010, 0.041
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2 \sigma(I_{obs})$, 4128
$N(param)_{refined}$:	372
Programs:	SHELX [1, 2], CrystalClear [3]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	U_{iso}^*/U_{eq}
Hg1	0.250000	0.14791(4)	0.750000	0.04013(12)
Hg2	0.500000	1.000000	0.500000	0.04030(12)
N1	0.1078(3)	0.1370(6)	0.6947(2)	0.0405(13)
N2	-0.0538(3)	0.1719(6)	0.6643(2)	0.0416(13)
N3	-0.1740(4)	0.3766(6)	0.6462(2)	0.0426(13)
N4	-0.2078(4)	0.4103(7)	0.5879(2)	0.0508(14)
N5	-0.2137(4)	0.5599(7)	0.5820(2)	0.0521(15)
N6	0.4880(3)	0.7826(6)	0.5346(2)	0.0351(12)
N7	0.4333(3)	0.5563(6)	0.5515(2)	0.0318(11)
N8	0.3115(4)	0.4306(6)	0.5964(2)	0.0375(12)
N9	0.3464(4)	0.3571(6)	0.6480(2)	0.0460(14)
N10	0.2862(4)	0.3863(7)	0.6836(3)	0.0539(16)
N11	0.5874(4)	1.1421(7)	0.6476(3)	0.0431(13)
N12	0.7412(5)	0.9757(7)	0.4929(3)	0.0564(17)
O1	0.3260(4)	0.0021(7)	0.6701(2)	0.0788(18)
H1	0.337950	0.039661	0.639985	0.095*
O2	0.5865(9)	1.0094(9)	0.6534(4)	0.176(4)
O3	0.6175(5)	1.2192(10)	0.6902(3)	0.132(3)
O4	0.5651(5)	1.1938(8)	0.5997(3)	0.112(3)
O5	0.6732(4)	0.9313(7)	0.4511(2)	0.0769(17)
O6	0.7156(4)	1.0127(6)	0.5389(2)	0.0722(16)
O7	0.8281(5)	0.9873(9)	0.4891(3)	0.123(3)
C1	0.0233(4)	0.1754(7)	0.7114(3)	0.0375(15)
H1A	0.018523	0.200658	0.749522	0.045*
C2	0.0813(5)	0.1101(8)	0.6349(3)	0.0541(19)
H2A	0.125545	0.081764	0.611491	0.065*
C3	-0.0166(5)	0.1305(9)	0.6157(3)	0.059(2)
H3A	-0.053003	0.119210	0.577276	0.071*
C4	-0.1579(4)	0.2177(7)	0.6634(3)	0.0460(17)
H4A	-0.203564	0.153275	0.635893	0.055*

Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
H4B	−0.171778	0.203158	0.702205	0.055*
C5	−0.1580(4)	0.5092(7)	0.6792(3)	0.0377(15)
C6	−0.1211(5)	0.5375(8)	0.7395(3)	0.0518(18)
H6A	−0.101634	0.459759	0.767018	0.062*
C7	−0.1164(5)	0.6905(9)	0.7539(3)	0.060(2)
H7A	−0.093430	0.717027	0.793203	0.072*
C8	−0.1442(5)	0.8094(8)	0.7130(3)	0.0561(19)
H8A	−0.140314	0.910687	0.725951	0.067*
C9	−0.1769(5)	0.7788(8)	0.6540(3)	0.0532(18)
H9A	−0.193301	0.857239	0.626474	0.064*
C10	−0.1844(4)	0.6246(8)	0.6375(3)	0.0407(16)
C11	0.4129(4)	0.6843(7)	0.5196(2)	0.0338(14)
H11A	0.354665	0.701770	0.491186	0.041*
C12	0.5596(4)	0.7129(7)	0.5784(3)	0.0391(15)
H12A	0.620290	0.756122	0.597385	0.047*
C13	0.5260(4)	0.5715(8)	0.5886(3)	0.0442(16)
H13A	0.558927	0.499120	0.615368	0.053*
C14	0.3665(4)	0.4223(7)	0.5499(3)	0.0363(14)
H14A	0.319546	0.418655	0.512057	0.044*
H14B	0.406039	0.328815	0.554161	0.044*
C15	0.2263(5)	0.5134(7)	0.5987(3)	0.0417(16)
C16	0.1643(5)	0.6106(9)	0.5594(4)	0.066(2)
H16A	0.174773	0.628292	0.521710	0.079*
C17	0.0863(6)	0.6798(10)	0.5789(4)	0.090(3)
H17A	0.043226	0.746598	0.554358	0.108*
C18	0.0721(6)	0.6488(11)	0.6363(5)	0.091(3)
H18A	0.018504	0.695660	0.648129	0.110*
C19	0.1327(6)	0.5539(10)	0.6752(4)	0.072(3)
H19A	0.122048	0.536118	0.712770	0.086*
C20	0.2126(5)	0.4843(7)	0.6552(3)	0.0472(18)
C21	0.3567(8)	−0.1480(11)	0.6761(5)	0.111(4)
H21A	0.381793	−0.178296	0.642327	0.166*
H21B	0.408906	−0.158580	0.710940	0.166*
H21C	0.301042	−0.212203	0.679380	0.166*

Experimental details

Hydrogen atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 (aromatic) or 0.96 Å (CH₃) or 0.97 Å (CH₂) and O—H = 0.82 Å. Hydrogen atoms were refined with *U*_{iso}(H) = 1.5 *U*_{eq}(C) for methyl H atoms and 1.2 *U*_{eq}(C, O) otherwise.

Comment

It is known that inorganic or organic counter anions can influence the coordination mode of the organic ligands and thus, influence the architectures and physical properties of the final products [4–8]. For example, two complexes with different compositions and structures can be obtained by the reaction of 1,4-benzenedicarboxylic acid and 2-(1*H*-imidazol-1-methyl)-1*H*-benzimidazole with CdCl₂ or CdBr₂ [9]. Yao reported a series of Cd(II) complexes by effective control of the

anions [4]. Self-assembly of 1-((benzotriazol-1-yl)methyl)-1*H*-1,3-imidazole (bmi) with HgCl₂ or HgBr₂ or HgI₂ results in the formation of [Hg(bmi)Cl₂]₂, [Hg(bmi)₂Br₂], and [Hg(bmi)₂I₂] [10, 11]. In order to further explore the influence of counter anions on the formation of complexes, we were motivated to synthesize a new Hg(II) complex [Hg(bmi)₂(CH₃OH)] · 2NO₃]_n by using bmi and Hg(NO₃)₂ as starting materials.

The asymmetric unit comprises two crystallographically independent halves of Hg(II) ions, two crystallographically independent bmi ligands, one coordinating methanol molecule and two uncoordinating nitrate anions. Each Hg1 ion is coordinated by four N atoms from four bmi ligands and by two O atoms from two methanol molecules resulting in a distorted octahedral geometry. Whereas each Hg2 ion is two-coordinated by two N atoms from two bmi ligands. The Hg—O bond length is 2.642(5) Å and Hg—N distances range from 2.076(5) to 2.695(6) Å, respectively; these values are comparable to distances reported in the literature for Hg(II) complexes [10, 12–14]. There are two kinds of crystallographically independent bmi ligands. One bmi ligand coordinates to Hg(II) in the monodentate mode through the nitrogen atom of the imidazole ring [15]. The other bmi ligand coordinates to two Hg(II) ions as bridging ligand through the nitrogen atoms of imidazole and benzotriazole rings. Hg1 and Hg2 ions are connected by bridging bmi ligands to form an one-dimensional chain with Hg1–Hg2 distance of 10.4438(16) Å. In addition, there is one O—H ··· O hydrogen bond, two C—H ··· N hydrogen bonds and eight C—H ··· O hydrogen bonds. Adjacent chains are linked by the mentioned hydrogen bonds, leading to a three-dimensional supramolecular architecture in the solid state.

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