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Crystal structure of bis(1-((2-ethyl-4-methyl-1*H*-imidazol-1-yl)methyl)-1*H*-benzo[d][1,2,3]triazole- κ^2 N:N')tetraiodidodicadmium(II), [Cd₂(C₁₃H₁₅N₅)₂I₄]

Figure 1: View of the title complex, showing the labeling of the 30% probability ellipsoids.

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Abstract

[Cd₂(C₁₃H₁₅N₅)₂I₄], triclinic, $P\bar{1}$ (no. 2), $a = 8.1348(16)$ Å, $b = 10.1716(17)$ Å, $c = 11.645(3)$ Å, $\alpha = 76.485(18)^\circ$, $\beta = 77.750(19)^\circ$, $\gamma = 74.030(16)^\circ$, $V = 889.4(3)$ Å³, $Z = 1$, $R_{\text{gt}}(F) = 0.0597$, $wR_{\text{ref}}(F^2) = 0.1251$, $T = 293(2)$ K.

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Table 1: Data collection and handling.

Crystal:	Colorless
Size:	0.20 × 0.18 × 0.17 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	4.7 mm ⁻¹
Diffractometer, scan mode:	Xcalibur, Eos, Gemini, ω -scans
θ_{max} , completeness:	29.4°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	7726, 7726
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 4831
$N(\text{param})_{\text{refined}}$:	193
Programs:	CrysAlis ^{PRO} [1], SHELX [2], OLEX2 [3]

The crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of materials

All starting materials are commercially available, and are used without further purification. 1-[(2-Ethyl-4-methyl-1*H*-imidazol-1-yl)methyl]-1*H*-benzotriazole (emimb) was prepared according to the literature method [4].

The ligand 1-[(2-ethyl-4-methyl-1*H*-imidazol-1-yl)methyl]-1*H*-benzotriazole (0.04 mmol, 0.0096 g) in methanol (6 mL) was added dropwise to a methanol solution (6 mL) of CdI₂ (0.04 mmol, 0.0146 g) in methanol. The resulting solution was allowed to stand at room temperature. After 3 weeks colourless crystals were obtained.

Experimental details

H atoms were generated geometrically and refined as riding atoms with C–H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2$ times $U_{\text{eq}}(\text{C})$ for aromatic H atoms, with C–H = 0.97 Å and $U_{\text{iso}}(\text{H}) = 1.2$ times $U_{\text{eq}}(\text{C})$ for methylene H atoms, and with C–H = 0.96 Å and $U_{\text{iso}}(\text{H}) = 1.5$ times $U_{\text{eq}}(\text{C})$ for methyl H atoms. The measured crystal was a non-merohedral twin (twin matrix $-1 \ 0 \ 0 \ 0 \ -1 \ 0 \ -0.458 \ -0.434 \ 1$).

Comment

Complexes based on multidentate *N*-heterocyclic ligands involving imidazole, triazole, benzimidazole or benzotriazole have attracted unparalleled attention owing to their intriguing molecular topologies and potential applications in

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

Atom	x	y	z	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
Cd1	0.19118(11)	0.70944(9)	0.25513(7)	0.0306(2)
I1	0.01426(12)	0.67877(10)	0.09371(7)	0.0473(3)
I2	0.51594(12)	0.54025(10)	0.24164(9)	0.0493(3)
N1	0.2196(13)	0.9367(10)	0.2159(8)	0.037(3)
N2	0.0756(13)	1.0289(11)	0.2346(8)	0.035(2)
N3	0.1084(12)	1.1557(10)	0.2058(7)	0.029(2)
N4	−0.0115(13)	1.2893(9)	0.3616(8)	0.033(2)
N5	−0.0571(12)	1.2848(9)	0.5539(7)	0.027(2)
C1	0.3526(16)	1.0044(13)	0.1745(9)	0.032(3)
C2	0.2829(15)	1.1432(12)	0.1682(9)	0.028(3)
C3	0.3823(18)	1.2453(15)	0.1266(11)	0.052(4)
H3	0.3326	1.3400	0.1215	0.062*
C4	0.5552(17)	1.1942(15)	0.0948(10)	0.046(4)
H4	0.6255	1.2563	0.0621	0.055*
C5	0.6335(18)	1.0456(15)	0.1104(12)	0.054(4)
H5	0.7533	1.0144	0.0952	0.065*
C6	0.5314(17)	0.9503(14)	0.1478(10)	0.039(3)
H6	0.5791	0.8551	0.1548	0.047*
C7	−0.0235(14)	1.2730(11)	0.2421(9)	0.028(3)
H7A	−0.1370	1.2593	0.2423	0.034*
H7B	−0.0101	1.3572	0.1850	0.034*
C8	0.1276(15)	1.3248(12)	0.3869(10)	0.032(3)
H8	0.2229	1.3451	0.3323	0.038*
C9	0.1002(15)	1.3248(12)	0.5033(10)	0.034(3)
C10	−0.1181(15)	1.2645(12)	0.4662(9)	0.029(3)
C11	0.2133(16)	1.3470(14)	0.5756(11)	0.046(3)
H11A	0.2618	1.2599	0.6236	0.069*
H11B	0.1474	1.4111	0.6268	0.069*
H11C	0.3050	1.3845	0.5240	0.069*
C12	−0.2846(14)	1.2197(13)	0.4772(12)	0.042(3)
H12A	−0.3404	1.2696	0.4085	0.051*
H12B	−0.3615	1.2472	0.5480	0.051*
C13	−0.2633(19)	1.0643(15)	0.4853(12)	0.055(4)
H13A	−0.2135	1.0401	0.4084	0.083*
H13B	−0.3744	1.0422	0.5102	0.083*
H13C	−0.1884	1.0127	0.5425	0.083*

ion exchange, magnetism, catalysis and biomedicine [5–10]. Recently, we have focused our attention on the design and synthesis the unsymmetrical *N*-heterocyclic ligand 1-[(2-ethyl-4-methyl-1*H*-imidazol-1-yl)methyl]-1*H*-benzotriazole (emimb).

The title compound forms a dinuclear structure. As is shown in the figure, the Cd(II) atom is four-coordinated by two N atoms from two bridging 1-[(2-ethyl-4-methyl-1*H*-imidazol-1-yl)methyl]-1*H*-benzotriazole (emimb) ligands, and two I atoms in a distorted tetrahedral coordination environment (with Cd–N bond lengths of 2.315(10) and 2.266(8) Å, and Cd–I bond lengths of 2.7149(13) and 2.7229(13) Å). The bond angles around Cd(II) ion range from 94.5(3) to 119.1(2)°. The Cd(II)

atoms are connected by the emimb ligands, leading to a cyclic dimer. The distance between two Cd atoms bridged by the emimb ligand is 8.675 Å. In addition, the imidazol rings in adjacent chains are parallel, with an average interplanar distance of 3.446 Å. So the crystal structure involves π – π interactions.

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