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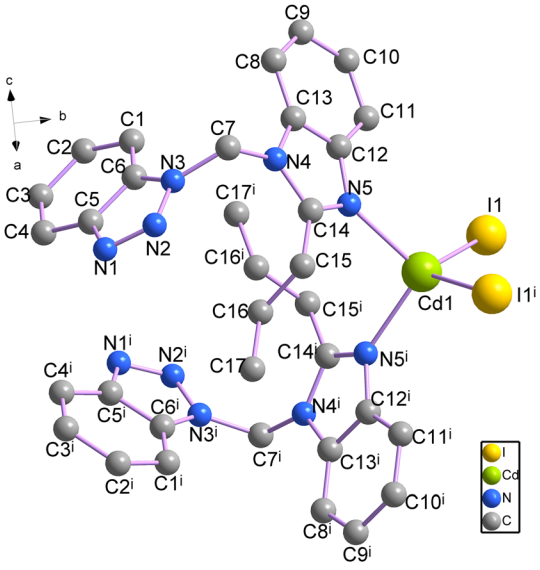
Crystal structure of diiodo-bis(1-((2-propyl-1*H*-benzo[d]imidazol-1-yl)methyl)-1*H*-benzo[d][1,2,3]triazole-κ^1*N*)cadmium(II), $C_{34}H_{34}CdI_2N_{10}$



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Abstract

$C_{34}H_{34}CdI_2N_{10}$, monoclinic, *C*2/*c* (no. 15), *a* = 17.1805(4) Å, *b* = 12.8107(2) Å, *c* = 17.6543(4) Å, *β* = 113.821(3)°, *Z* = 4, *V* = 3554.59(15) Å^3, $R_{gt}(F)$ = 0.0447, $wR_{ref}(F^2)$ = 0.1192, T = 293(2) K.

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The molecular structure is shown in the figure. Table 1 contains the crystallographic data and the list of the atoms including atomic coordinates and displacement parameters can be found in the cif-file attached to this article.

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Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.23 × 0.20 × 0.13 mm
Wavelength:	CuKα radiation (1.54184 Å)
μ:	18.9 mm^{-1}
Diffractometer, scan mode:	Xcalibur, Eos, *ω* scans
θ_{max}, completeness:	70.9°, 100 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	6751, 3343, 0.039
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 2,915
$N(param)_{refined}$:	214
Programs:	Rigaku,[1] SHELX,[2] OLEX[3]

1 Source of materials

All starting materials are commercially available without further purification. 1-[(2-propyl-1-*H*-benzimidazole-1-yl) methyl]-1*H*-benzotriazole (pbmb) was prepared according to the literature method with some modifications.[4] The ligand 1-[(2-propyl-1-*H*-benzimidazole-1-yl)methyl]-1*H*-benzotriazole (0.02 mmol, 0.0117 g) was dissolved in 2 mL of methanol solution and the solution was slowly added to 2 ml of CdI_2 (0.02 mmol, 0.0097 g) of methanol solution. The prepared solution was placed at room temperature and colorless crystals were obtained after one weeks.

2 Experimental details

H atoms were generated geometrically and refined as riding atoms with C–H = 0.93 Å and the U_{iso}(H) = 1.2 times U_{eq}(C) for aromatic H atoms, with C–H = 0.97 Å and U_{iso}(H) = 1.2 times U_{eq}(C) for methylene H atoms, and with C–H = 0.96 Å and U_{iso}(H) = 1.5 times U_{eq}(C) for methyl H atoms.

3 Comment

Research has shown that nitrogen-containing compounds such as pyrazoles, benzimidazole and triazoles are easily coordinated with metal ions,[5] such as Zn(II),[6] Ag(I) etc., thereby enhancing the stability and activity of the complexes.[7,8] For example, triazole metal complexes have antibacterial activity.

The Desai teams synthesized benzotriazole ligands and coordinated them with transition metals such as Cu(II), Ni(II), and Co(II), the Cu(II) complexes was found to exhibit the highest antibacterial activity.[9] The Wang team synthesized four novel copper metal complexes with triazoles and found that they have good hypoglycemic activity, they also studied the structure-activity relationship between the complexes and hypoglycemic activity.[10] Cadmium, as a heavy metal, exhibits inhibition of proteasome activity in tumor cells after coordinating with nitrogen-containing heterocycles, thereby inducing specific apoptosis of cancer cells.[11] In addition, the lipophilicity of cadmium complexes enhances their ability to penetrate bacterial membranes, which helps overcome the resistance of traditional antibiotics.[12,13]

X-ray crystallographic analysis shows that the title complex is mononuclear with a symmetric structure. As shown in the Figure, the central atom Cd(II) is coordinated with two I- ligands (I1 and I1i) and two N atoms (N5 and N5i) from two crystallogaphically dependent pbmb ligands, respectively. The Cd–I and Cd–N bonds around Cd1 are of length: Cd1–I1: 2.7389 (5) Å; Cd1–I1i: 2.7389 (5) Å; Cd1–N5: 2.282 (4) Å; Cd1–N5i: 2.282 (4) Å. The range of bond angles around the metal center Cd(II) is 102.4 (2)° –113.6 (3)°. The smallest bond angle is N5i–Cd1–N5, and the largest bond angle is I1i–Cd1–I1. In each pbmb ligand, the angle between the benzotriazole and the benzimidazole ring is 79.1°. The two adjacent benzimidazole rings have π-π conjugation, and the distance between the surface centers is 3.7515 Å. Two adjacent benzotriazoles also have π-π conjugation with a distance of 3.7090 Å between the centers of the faces. Bond lengths and angles are all in the expected ranges.[14]

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