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Crystal structure of Bis{1-[(benzotriazol-1-yl)methyl]-1-*H*-1,3-(2-methylimidazol)}diiodidocadmium(II), [Cd(C₁₁H₁₁N₅)₂I₂], C₂₂H₂₂N₁₀I₂Cd

Abstract

C₂₂H₂₂N₁₀I₂Cd, triclinic, $P\bar{1}$ (no. 2), $a = 10.5476(8)$ Å, $b = 11.1759(9)$ Å, $c = 12.7735(10)$ Å, $\alpha = 103.372(7)^\circ$, $\beta = 105.811(7)^\circ$, $\gamma = 100.270(6)^\circ$, $V = 1361.85(18)$ Å³, $Z = 2$, $R_{\text{gt}}(F) = 0.0324$, $wR_{\text{ref}}(F^2) = 0.0661$, $T = 291(2)$ 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.

Table 1: Data collection and handling.

Crystal:	Colourless
Size:	0.18 × 0.16 × 0.15 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	3.10 mm ⁻¹
Diffractometer, scan mode:	Xcalibur, Eos, ω
θ_{max} , completeness:	26.4°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	11352, 5559, 0.024
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 4420
$N(\text{param})_{\text{refined}}$:	318
Programs:	CrysAlis ^{PRO} [1], Olex2 [2], SHELX [3]

Source of material

A methanol solution (4 mL) of KSCN (0.1 mmol) was added dropwise into a methanol solution (2 mL) of CdI₂ (0.05 mmol), giving a clear solution. 1-((Benzotriazol-1-yl)methyl)-1-*H*-1,3-(2-methylimidazol) (0.1 mmol) in 4 mL of methanol was added to the above solution. The resulting solution was left at room temperature. After five days, colorless crystals were obtained and dried in air.

Experimental details

H atoms were generated geometrically, with C–H = 0.96, 0.97 and 0.93 Å for methyl, methylene and aromatic H, respectively, and constrained to ride on their parent atoms.

Discussion

Coordination compounds have attracted interest for potential applications in various areas [4]. The multidentate *N*-heterocyclic ligands containing rich coordination sites, such

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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}
I1	0.19121(3)	0.59324(3)	0.63816(3)	0.05157(10)
I2	0.49783(3)	0.91981(3)	0.61728(3)	0.05145(10)
Cd1	0.45876(3)	0.72067(3)	0.70322(2)	0.03531(9)
N1	0.5325(3)	0.7962(3)	0.8956(3)	0.0371(8)
N2	0.6326(3)	0.9252(3)	1.0689(3)	0.0356(8)
N3	0.8528(3)	1.0031(3)	1.2178(3)	0.0405(8)
N4	0.9700(4)	1.0630(4)	1.2056(3)	0.0520(10)
N5	1.0717(3)	1.0319(4)	1.2667(3)	0.0564(10)
N6	0.6062(3)	0.6085(3)	0.6713(3)	0.0404(8)
N7	0.7301(3)	0.4706(3)	0.6683(3)	0.0432(9)
N8	0.8199(3)	0.3355(3)	0.7769(3)	0.0440(9)
N9	0.7281(4)	0.2864(4)	0.8231(4)	0.0623(11)
N10	0.7937(4)	0.2725(4)	0.9188(4)	0.0681(12)
C1	0.4548(4)	0.7701(4)	0.9631(4)	0.0423(10)
H1	0.3730	0.7078	0.9383	0.051*
C2	0.5150(4)	0.8479(4)	1.0695(4)	0.0469(11)
H2	0.4840	0.8497	1.1312	0.056*
C3	0.6402(4)	0.8914(4)	0.9620(3)	0.0333(9)
C4	0.7523(4)	0.9525(4)	0.9282(4)	0.0485(11)
H4A	0.7625	1.0427	0.9482	0.073*
H4B	0.7317	0.9192	0.8475	0.073*
H4C	0.8355	0.9352	0.9671	0.073*
C5	0.7260(4)	1.0301(4)	1.1652(4)	0.0444(10)
H5A	0.7455	1.1044	1.1397	0.053*
H5B	0.6816	1.0505	1.2218	0.053*
C6	0.8816(4)	0.9326(4)	1.2911(3)	0.0386(9)
C7	1.0225(4)	0.9524(4)	1.3215(4)	0.0435(10)
C8	1.0908(5)	0.8992(4)	1.4013(4)	0.0559(12)
H8	1.1851	0.9129	1.4239	0.067*
C9	1.0133(6)	0.8264(5)	1.4450(4)	0.0644(14)
H9	1.0560	0.7890	1.4980	0.077*
C10	0.8728(5)	0.8065(5)	1.4126(4)	0.0611(13)
H10	0.8242	0.7561	1.4446	0.073*
C11	0.8030(5)	0.8582(4)	1.3354(4)	0.0504(11)
H11	0.7087	0.8443	1.3139	0.061*
C12	0.7343(4)	0.6670(4)	0.6725(4)	0.0451(11)
H12	0.7632	0.7515	0.6748	0.054*
C13	0.8103(4)	0.5821(5)	0.6698(4)	0.0488(12)
H13	0.8996	0.5964	0.6690	0.059*
C14	0.6062(4)	0.4894(4)	0.6687(4)	0.0414(10)
C15	0.4902(4)	0.3913(5)	0.6651(5)	0.0727(17)
H15A	0.4829	0.3125	0.6112	0.109*
H15B	0.4077	0.4177	0.6424	0.109*
H15C	0.5044	0.3798	0.7392	0.109*
C16	0.7698(5)	0.3517(4)	0.6648(4)	0.0528(12)
H16A	0.6918	0.2811	0.6179	0.063*
H16B	0.8403	0.3497	0.6296	0.063*
C17	0.9492(4)	0.3535(4)	0.8469(3)	0.0380(9)
C18	0.9308(5)	0.3122(4)	0.9362(4)	0.0479(11)
C19	1.0428(6)	0.3117(5)	1.0256(4)	0.0663(14)
H19	1.0309	0.2836	1.0861	0.080*
C20	1.1672(6)	0.3531(5)	1.0206(5)	0.0715(15)
H20	1.2432	0.3536	1.0786	0.086*
C21	1.1853(5)	0.3962(5)	0.9289(5)	0.0683(15)
H21	1.2735	0.4254	0.9287	0.082*
C22	1.0774(4)	0.3965(4)	0.8398(4)	0.0528(12)
H22	1.0895	0.4237	0.7789	0.063*

as imidazole, triazole, tetrazole are often employed to produce different polymeric networks due to their various coordination modes [4–8]. Recently, our group synthesized 1-[(benzotriazol-1-yl)methyl]-1-*H*-1,3-(2-methyl-imidazol)(bmi) and studied its coordination behavior [9–12]. To study the effect of subsidiary ligands on the coordination behavior of bmi, we used bmi in the presence of KSCN. Single crystal X-ray diffraction indicated that the ion SCN coordinated metal ions in some complexes and didn't in others. At the same time, in some complexes where the ion SCN[−] didn't coordinate the metal, the cell parameters of complexes are different to those of the complexes that were obtained with and without KSCN.

Similarly to the reported compound [9], the title compound is a mononuclear structure. As is shown in the upper part of the figure, the Cd(II) atom is four-coordinated by two N atoms and two iodides. But the title compound belongs to the triclinic system, differently to the reported compound, which is monoclinic. Cd–N bond lengths are 2.263(3) Å and 2.228(3) Å, and Cd–I bond lengths are 2.7247(5) Å and 2.7162(4) Å, respectively. The bond angles around the Cd atom vary from 102.30(11)° (N6–Cd1–N1) to 117.88(9)° (N6–Cd1–I1). The dihedral angle between the imidazole planes in the ligand is 104.9°, which is different to that of the reported compound (75.4°). In the crystal, adjacent molecules are stacked through the benzotriazol π–π interactions (the centroid-centroid distance is 3.763 Å and 4.223 Å, respectively) (figure bottom) [13].

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References

- Agilent Technologies: CrysAlis PRO Software system, version 1.171.35.15, Agilent Technologies UK Ltd, Oxford, UK (2011).
- Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H.: A complete structure solution, refinement and analysis program. *J. Appl. Crystallogr.* **42** (2009) 339–341.
- Sheldrick, G. M.: A short history of SHELX. *Acta Crystallogr. A* **64** (2008) 112–122.
- Ma, K.; Zhao, X.-N.; Han, X.; Ding, J.; Meng, X.-R.; Hou, H.-W.: Interesting pH-responsive behavior in benzothiadiazole-derived coordination polymer constructed via an *in situ* click synthesis. *Cryst. Growth Des.* **18** (2018) 7419–7425.
- Yang, H.-Y.; Li, L.-K.; Wu, J.; Hou, H.-W.; Xiao, B.; Fan, Y.-T.: 3D Coordination framework with uncommon two-fold interpenetrated {3³·5⁹·6³}-lcy net and coordinated anion exchange. *Chem. Eur. J.* **15** (2009) 4049–4056.
- Seth, S.; Matzger, A. J.: Coordination polymerization of 5,5'-dinitro-2*H*,2*H'*-3,3'-bi-1,2,4-triazole leads to a dense explosive with high thermal stability. *Inorg. Chem.* **56** (2017) 561–565.

7. Liu, L.; Huang, C.; Xue, X.-N.; Li, M.; Hou, H.-W.; Fan, Y.-T.: Ni(II) coordination polymers constructed from the flexible tetracarboxylic acid and different *N*-Donor ligands: structural diversity and catalytic activity. *Cryst. Growth Des.* **15** (2015) 4507–4517.
8. Yang, Y.; Jiang, F. L.; Liu, C. P.; Chen, L.; Gai, Y. L.; Pang, J. D.; Su, K. Z.; Wan, X. Y.; Hong, M. C.: Self-assembly syntheses, structural characterization, and luminescent properties of lanthanide coordination polymers constructed by three triazole-carboxylate ligands. *Cryst. Growth Des.* **16** (2016) 2266–2276.
9. Yang, H.-Y.; Li, Y.-H.; Chen, H.: Crystal structure of bis{1-[(benzotriazol-1-yl)methyl]-1-*H*-1,3-(2-methyl-imidazol)} diiodido-cadmium(II), $[Cd(C_{11}H_{11}N_5)_2I_2]$, $C_{22}H_{22}CdI_2N_{10}$. *Z. Kristallogr. NCS* **227** (2012) 527–528.
10. Yang, H.-Y.; Li, Y.-H.: Crystal structure of bis{1-[(benzotriazol-1-yl)methyl]-1-*H*-1,3-(2-methyl-imidazol)}dibromidomercury(II), $[Hg(C_{11}H_{11}N_5)_2Br_2]$, $C_{22}H_{22}HgBr_2N_{10}$. *Z. Kristallogr. NCS* **229** (2014) 83–84.
11. Yang, H.-Y.: Crystal structure of aquadichloridobis(1-((2-methyl-1*H*-imidazol-1-yl)methyl)-1*H*-benotriazole- κN)mercury(II), $C_{22}H_{24}HgCl_2N_{10}O$. *Z. Kristallogr. NCS* **231** (2016) 687–688.
12. Yang, H.-Y.; Zhao, Y.-M.; He, F.; Li, H.; Wang, H.-F.; Li, Y.-H.: Crystal structure of bis{1-[(benzotriazol-1-yl)-methyl]-1-*H*-1,3-(2-methyl-imidazol)- κN }-dithiocyno- κN -zinc(II), $C_{24}H_{22}ZnS_2N_{12}$. *Z. Kristallogr. NCS* **233** (2018) 839–841.
13. Janiak, C.: A critical account on π – π stacking in metal complexes with aromatic nitrogen-containing ligands. *Dalton Trans.* (2000) 3885–3896.