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Crystal structure of poly[dibromido-bis(μ_2 -1,6-di(1*H*-imidazol-1-yl)hexane- $\kappa^2 N:N'$)cadmium(II)], $C_{24}H_{36}Br_2N_8Cd$

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Abstract

$C_{24}H_{36}Br_2N_8Cd$, monoclinic, $P2_1/c$ (no. 14), $a = 9.6915(4)$ Å, $b = 7.6614(2)$ Å, $c = 19.0851(8)$ Å, $\beta = 100.529(4)^\circ$, $V = 1393.21(9)$ Å³, $Z = 2$, $R_{gt}(F) = 0.0744$, $wR_{ref}(F^2) = 0.1823$, $T = 293(2)$ K.

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The asymmetric unit of the polymeric title structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

A mixture of $Cd(NO_3)_2 \cdot 2H_2O$ (0.1 mmol, 0.0272 g), 1,6-di(1*H*-imidazol-1-yl)hexane (1,6-dih) (0.2 mmol, 0.0612 g), HBr (0.1 mmol/mL, 2 mL), was dissolved in 9 mL H_2O . Then the solution was heated in a 23 mL Teflon-lined autoclave under autogenous pressure at 373 K for 4 days. After cooling to room

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	$0.42 \times 0.38 \times 0.26$ mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	3.68 mm^{-1}
Diffractometer, scan mode:	EosS2, ω
θ_{max} , completeness:	25.5° , >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int} :	29900, 2585, 0.084
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2 \sigma(I_{obs})$, 2356
$N(param)_{refined}$:	160
Programs:	CrysAlis ^{PRO} [1], SHELX [2, 3]

temperature crystals formed. The colourless crystals suitable for X-ray diffraction analysis were collected.

Experimental details

Coordinates of hydrogen atoms were included using riding models (AFIX 23 and AFIX 43 [3]). Their U_{iso} values were set to $1.2U_{eq}$ of the parent atoms.

Comment

The design and construction of metal-organic frameworks (MOFs) is the hottest research in the last decade. The organic ligands, which have their differences in the size, the exibility, the coordination ability, the number of the *N*-donor ligands, such as 1,6-bis(1,2,4-triazol-1-yl)hexane, have significant influence on structure of final product [4]. The flexibility of *N*-donor ligands can result not only in gauche and anti conformations in coordination, but also in free rotation to

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

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
Cd1	1.0000	1.0000	0.5000	0.0342(3)
N1	0.9210(7)	0.8669(9)	0.3905(3)	0.0282(15)
N2	0.2051(7)	−0.3326(9)	0.0207(4)	0.0305(16)
N3	0.8798(7)	0.6851(9)	0.3003(4)	0.0287(15)
N4	0.3487(7)	−0.1193(9)	0.0619(4)	0.0280(15)
Br1	0.86144(11)	0.73774(13)	0.57319(6)	0.0473(3)
C1	0.8350(10)	0.9451(12)	0.3351(5)	0.036(2)
H1	0.7997	1.0578	0.3356	0.043 [*]
C2	0.8086(9)	0.8336(12)	0.2787(5)	0.036(2)
H2	0.7531	0.8550	0.2343	0.044 [*]
C3	0.9464(9)	0.7094(11)	0.3678(4)	0.0285(18)
H3	1.0028	0.6265	0.3948	0.034 [*]
C4	0.8764(9)	0.5245(12)	0.2582(5)	0.037(2)
H4A	0.9293	0.4343	0.2870	0.044 [*]
H4B	0.9208	0.5458	0.2174	0.044 [*]
C5	0.7289(10)	0.4622(13)	0.2328(6)	0.046(3)
H5A	0.6770	0.5541	0.2045	0.055 [*]
H5B	0.6853	0.4434	0.2740	0.055 [*]
C6	0.7149(9)	0.2971(12)	0.1890(5)	0.036(2)
H6A	0.7665	0.3102	0.1503	0.043 [*]
H6B	0.7563	0.2009	0.2186	0.043 [*]
C7	0.5651(10)	0.2547(13)	0.1588(6)	0.047(3)
H7A	0.5298	0.3412	0.1229	0.057 [*]
H7B	0.5109	0.2652	0.1966	0.057 [*]
C8	0.5391(9)	0.0740(12)	0.1255(5)	0.037(2)
H8A	0.6051	0.0531	0.0938	0.044 [*]
H8B	0.5546	−0.0139	0.1626	0.044 [*]
C9	0.3931(9)	0.0587(11)	0.0847(5)	0.035(2)
H9A	0.3292	0.1038	0.1140	0.041 [*]
H9B	0.3844	0.1322	0.0427	0.041 [*]
C10	0.2153(9)	−0.1685(11)	0.0406(5)	0.0307(18)
H10	0.1387	−0.0951	0.0400	0.037 [*]
C11	0.3402(10)	−0.3922(12)	0.0294(5)	0.039(2)
H11	0.3665	−0.5045	0.0189	0.047 [*]
C12	0.4306(9)	−0.2609(12)	0.0561(5)	0.039(2)
H12	0.5279	−0.2672	0.0679	0.047 [*]

meet the requirements of the coordination geometry of the metal ions in the assembly process. The organic ligand 1,6-di(1*H*-imidazol-1-yl)hexane serves as bridging ligand [5–8].

In the title complex, there are one half of a Cd(II), one (1,6-dih) ligand, and one bromide in the asymmetric unit. The cadmium atom Cd1 is six-coordinated with a distorted octahedral geometry by four N atoms from the 1,6-dih ligands from the axial positions (see the figure). The Cd–Br bond length is 2.9121(11) Å; and the Cd–N ones are in the range of 2.325(6) to 2.338(7) Å, respectively. The bond angles of N–Cd–N are in the range of 87.6(2)° to 180°.

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