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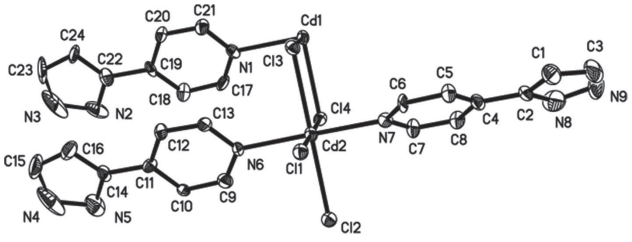
Crystal structure of *catena*-poly[hexakis(μ_2-chlorido)-hexakis(4-(1H-pyrazol-5-yl)pyridine-κ*N*)tricadmium(II)], $Cd_3C_{48}H_{42}Cl_6N_{18}$



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Abstract

$Cd_3C_{48}H_{42}Cl_6N_{18}$, monoclinic, *C*2/*c* (no. 15), $a = 11.4564(7)$ Å, $b = 21.1547(15)$ Å, $c = 21.3475(13)$ Å, $\beta = 95.192(5)°$, $V = 5152.5(6)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0381$, $wR_{ref}(F^2) = 0.1152$, $T = 293(2)$ K.

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A part of the polymeric title 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 material

3-(4-Pyridyl)pyrazole (0.04 g, 0.3 mmol) and $CdCl_2$ (0.07 g, 0.4 mmol) were added to H_2O (10 mL) in a Teflon-lined stainless steel reactor. The mixture was heated at 393 K for 3 d, and then slowly cooled down to room temperature. Colorless block crystals of the title compound were obtained.

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Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.42 × 0.32 × 0.21 mm
Wavelength:	Mo *Kα* radiation (0.71073 Å)
μ:	15.9 cm^{-1}
Diffractometer, scan mode:	Bruker FRAMBO, φ and ω
$2\theta_{max}$, completeness:	51°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	14107, 4780, 0.028
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1412
$N(param)_{refined}$:	340
Programs:	SHELX [16], Bruker programs [17]

Experimental details

The hydrogen atoms were placed at calculated positions with the SHELX program (AFIX options: 43 and 147) [16].

Discussion

Coordination polymers (CPs) have attracted worldwide attention not only for their potential applications in the fields of photochemical areas [1], gas adsorption and separation [2], molecular magnetism [3], heterogeneous catalysis [4, 5], and nonlinear optics [6] but also for their intriguing topologies and crystal packing motifs [7–9]. However, it is still a challenge to exactly predict the structure of CPs. The self-assembly processes of CPs are influenced by many factors, such as organic ligands [8–10], pH value [11], solvent, temperature, and reagent concentration [12–15]. In recent years, non-covalent interactions, such as hydrogen-bonding and ionic interactions between building units are also considered as important factors in the self-organization of the frameworks. N-donor ligands have been to date the most popular choice for the construction of divalent metal CPs, wherein the geometric disposition of the N-donor ligands and their numerous possible binding modes play a crucial role in structure formation, in tandem with coordination geometry preferences.

The crystal structure of the title compound comprises two crystallographically independent Cd(II) cations, three 3-(4-Pyridyl)pyrazole ligands and three Cl atoms. The coordination geometry around both Cd(II) centers is best described as a

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

Atom	x	y	z	U_{iso}*/U_{eq}
Cd1	0.0000	0.12501(4)	0.7500	0.0312(2)
Cd2	0.33342(5)	0.12499(3)	0.74998(3)	0.03094(16)
Cl1	0.5000	0.03602(13)	0.7500	0.0328(6)
Cl2	0.5000	0.21384(13)	0.7500	0.0343(7)
Cl3	0.16720(16)	0.03600(8)	0.75010(9)	0.0319(4)
Cl4	0.16681(15)	0.21399(8)	0.75000(9)	0.0321(4)
N1	−0.0185(5)	0.1245(3)	0.6409(3)	0.0322(16)
N2	−0.0270(6)	0.1772(4)	0.4038(4)	0.075(3)
N3	−0.0517(8)	0.1529(8)	0.3435(4)	0.131(6)
H3	−0.0467	0.1736	0.3091	0.157*
N4	0.2830(8)	0.1539(7)	0.3459(5)	0.123(5)
H4	0.2920	0.1753	0.3124	0.148*
N5	0.3047(6)	0.1764(5)	0.4064(4)	0.076(3)
N6	0.3163(5)	0.1258(3)	0.6418(2)	0.0308(16)
N7	0.3520(5)	0.1247(3)	0.8582(3)	0.0298(15)
N8	0.3631(6)	0.1774(4)	1.0954(4)	0.079(3)
N9	0.3843(9)	0.1527(8)	1.1553(5)	0.135(6)
H9	0.3763	0.1728	1.1896	0.162*
C1	0.4186(7)	0.0740(5)	1.0949(5)	0.061(3)
H1	0.4369	0.0340	1.0805	0.074*
C2	0.3848(6)	0.1260(4)	1.0577(3)	0.0333(19)
C3	0.4201(9)	0.0909(8)	1.1514(6)	0.088(5)
H3A	0.4423	0.0653	1.1858	0.106*
C4	0.3741(6)	0.1246(4)	0.9900(3)	0.036(2)
C5	0.3961(6)	0.0710(4)	0.9546(3)	0.0379(19)
H5	0.4189	0.0333	0.9746	0.045*
C6	0.3840(6)	0.0746(4)	0.8907(3)	0.038(2)
H6	0.3998	0.0383	0.8684	0.045*
C7	0.3300(6)	0.1778(4)	0.8910(3)	0.043(2)
H7	0.3075	0.2145	0.8692	0.051*
C8	0.3402(6)	0.1785(4)	0.9555(3)	0.037(2)
H8	0.3242	0.2155	0.9766	0.044*
C9	0.3377(6)	0.1771(4)	0.6074(3)	0.039(2)
H9A	0.3617	0.2136	0.6291	0.046*
C10	0.3274(6)	0.1803(4)	0.5429(3)	0.037(2)
H10	0.3438	0.2176	0.5224	0.044*
C11	0.2917(6)	0.1263(4)	0.5088(3)	0.0305(18)
C12	0.2710(5)	0.0711(4)	0.5439(3)	0.036(2)
H12	0.2500	0.0334	0.5233	0.043*
C13	0.2822(6)	0.0736(4)	0.6077(4)	0.037(2)
H13	0.2654	0.0372	0.6296	0.044*
C14	0.2816(6)	0.1234(5)	0.4402(3)	0.038(2)
C15	0.2441(8)	0.0909(7)	0.3467(6)	0.090(5)
H15	0.2210	0.0662	0.3118	0.108*
C16	0.2462(7)	0.0738(5)	0.4045(5)	0.055(3)
H16	0.2267	0.0340	0.4190	0.066*
C17	0.0026(6)	0.1761(4)	0.6096(4)	0.041(2)
H17	0.0248	0.2125	0.6322	0.049*
C18	−0.0065(6)	0.1789(4)	0.5453(3)	0.041(2)
H18	0.0083	0.2167	0.5251	0.049*
C19	−0.0379(5)	0.1251(4)	0.5100(3)	0.033(2)
C20	−0.0630(6)	0.0714(4)	0.5443(4)	0.046(2)
H20	−0.0877	0.0346	0.5233	0.056*
C21	−0.0515(6)	0.0727(4)	0.6077(4)	0.040(2)
H21	−0.0673	0.0360	0.6294	0.048*
C22	−0.0511(7)	0.1236(5)	0.4389(4)	0.047(2)
C23	−0.0859(10)	0.0899(7)	0.3472(5)	0.088(5)
H23	−0.1051	0.0633	0.3131	0.106*
C24	−0.0866(6)	0.0746(5)	0.4046(4)	0.050(3)
H24	−0.1085	0.0355	0.4197	0.059*

distorted octahedral environment (*cf*. the figure). The coordination spheres around both six-coordinated Cd(II) centers is composed by two N atoms from two pyrazole ligands and four Cl atoms. Cl atoms act as a bridge linking neighboring Cd(II) ions to form a one-dimensional chain. The 1D chains are linked by N–H···Cl hydrogen bonding to generate a 3D supramolecular architecture.

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