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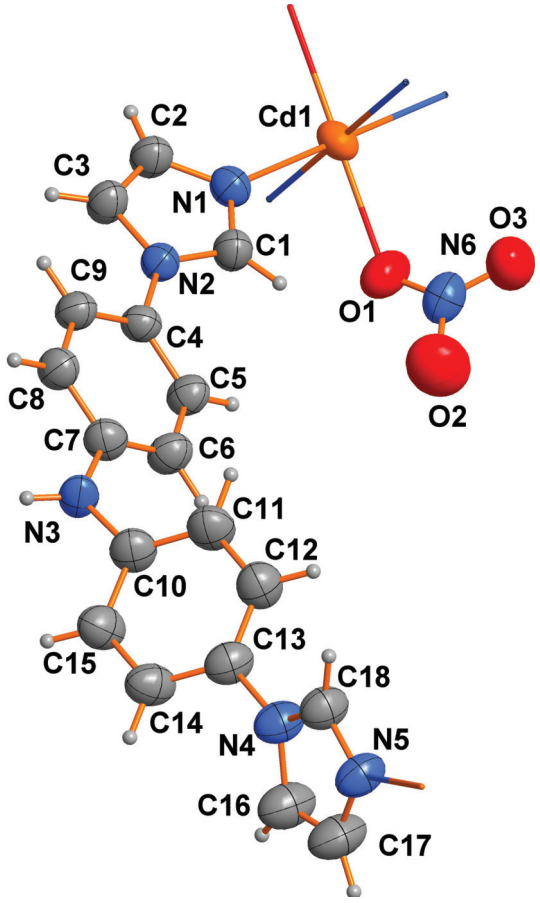
# Crystal structure of poly[bis(μ$_2$-bis(4-(1*H*-imidazol-1-yl)phenyl)amine-κ$^2$*N*:*N*′)-bis(nitrato-κ*O*)cadmium(II)], $C_{36}H_{30}CdN_{12}O_6$

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## Abstract

$C_{36}H_{30}CdN_{12}O_6$, monoclinic, $P2_1/c$ (no. 14), $a = 9.9673(10)$ Å, $b = 8.6759(9)$ Å, $c = 20.756(2)$ Å, $\beta = 98.926(7)°$, $V = 1773.1(3)$ Å$^3$, $Z = 2$, $R_{gt}(F) = 0.0554$, $wR_{ref}(F^2) = 0.1561$, $T = 2932$ K.

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A part of the molecular 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.

**Table 1:** Data collection and handling.

| | |
|---|---|
| Crystal: | Yellow block |
| Size: | 0.32 × 0.18 × 0.16 mm |
| Wavelength: | Mo *Kα* radiation (0.71073 Å) |
| $\mu$: | 0.68 mm$^{-1}$ |
| Diffractometer, scan mode: | Xcalibur, $\omega$ |
| $\theta_{max}$, completeness: | 27.5°, >99% |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$, $R_{int}$: | 27337, 4053, 0.062 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\ \sigma(I_{obs})$, 2984 |
| $N(param)_{refined}$: | 250 |
| Programs: | Olex2 [1], SHELX [2], CrysAlis$^{PRO}$ [3] |

## Source of material

A mixture of bis(4-(1*H*-imidazol-1-yl)phenyl)amine (2.5 mg), $Cd(NO_3)_2{\cdot}4\ H_2O$ (3.0 mg), and 6 mL mixed solution of EtOH/$H_2O$ ($v/v = 1/5$) was added to a hard glass tube, pumped to a near-vacuum, heated at 140 °C for 36 h, and cooled to room temperature with a decreasing rate of 2 °C/h. Colorless block crystals of 1 were obtained with the yield of *ca.* 37% (based on $Cd(NO_3)_2{\cdot}4\ H_2O$).

## Experimental details

H atoms bonded to C atoms from organic ligands were positioned geometrically and refined using a riding model, with C—H = 0.93 Å, with $U_{iso}(H) = 1.2$ times $U_{eq}(C)$.

## Comment

The containing *N*-ligands have been widely applied in the construction coordination polymers in recent years [4–6]. The recent studies prove that *N*-donor ligands can be acted as a good choice for preparing metal coordination polymers.

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

| Atom | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cd1 | 0.500000 | 0.500000 | 0.000000 | 0.05464(18) |
| O1 | 0.5979(4) | 0.2569(5) | 0.0136(2) | 0.0861(10) |
| O2 | 0.6743(6) | 0.0676(7) | 0.0739(3) | 0.1252(15) |
| O3 | 0.7800(4) | 0.2828(5) | 0.0788(3) | 0.1088(15) |
| N1 | 0.3118(3) | 0.3616(4) | 0.01984(18) | 0.0553(8) |
| N2 | 0.1874(3) | 0.1742(4) | 0.05040(16) | 0.0487(7) |
| N3 | 0.0296(3) | −0.3662(4) | 0.16040(18) | 0.0548(8) |
| H3 | −0.056302 | −0.384117 | 0.153088 | 0.066* |
| N4 | 0.3407(4) | −0.8096(5) | 0.30620(18) | 0.0635(9) |
| N5 | 0.4468(4) | −0.9331(5) | 0.39130(19) | 0.0652(9) |
| N6 | 0.6820(4) | 0.2070(6) | 0.0574(2) | 0.0722(10) |
| C1 | 0.3126(4) | 0.2250(5) | 0.0476(2) | 0.0575(9) |
| H1 | 0.391206 | 0.170431 | 0.063361 | 0.069* |
| C2 | 0.1783(4) | 0.3985(5) | 0.0032(2) | 0.0602(10) |
| H2 | 0.145890 | 0.488846 | −0.017743 | 0.072* |
| C3 | 0.1004(5) | 0.2858(5) | 0.0215(2) | 0.0596(10) |
| H3A | 0.006043 | 0.283511 | 0.015694 | 0.071* |
| C4 | 0.1505(4) | 0.0335(4) | 0.0786(2) | 0.0491(8) |
| C5 | 0.2397(4) | −0.0890(5) | 0.0869(2) | 0.0545(9) |
| H5 | 0.323871 | −0.081325 | 0.073143 | 0.065* |
| C6 | 0.2033(5) | −0.2239(5) | 0.1158(2) | 0.0597(9) |
| H6 | 0.263026 | −0.306893 | 0.121445 | 0.072* |
| C7 | 0.0793(4) | −0.2340(5) | 0.1360(2) | 0.0568(9) |
| C8 | −0.0101(4) | −0.1126(5) | 0.1271(2) | 0.0561(9) |
| H8 | −0.094627 | −0.120723 | 0.140531 | 0.067* |
| C9 | 0.0254(5) | 0.0211(5) | 0.0984(2) | 0.0545(9) |
| H9 | −0.035232 | 0.103211 | 0.092344 | 0.065* |
| C10 | 0.1148(5) | −0.4705(5) | 0.1963(2) | 0.0605(10) |
| C11 | 0.2229(5) | −0.4280(6) | 0.2415(2) | 0.0682(11) |
| H11 | 0.244873 | −0.324521 | 0.248329 | 0.082* |
| C12 | 0.2988(5) | −0.5404(6) | 0.2770(2) | 0.0661(11) |
| H12 | 0.373922 | −0.513294 | 0.307240 | 0.079* |
| C13 | 0.2636(5) | −0.6924(5) | 0.2675(2) | 0.0605(9) |
| C14 | 0.1530(5) | −0.7349(6) | 0.2241(2) | 0.0675(10) |
| H14 | 0.129190 | −0.838205 | 0.218639 | 0.081* |
| C15 | 0.0769(5) | −0.6226(6) | 0.1883(2) | 0.0676(11) |
| H15 | 0.000366 | −0.649546 | 0.158874 | 0.081* |
| C16 | 0.3789(7) | −0.9506(7) | 0.2845(3) | 0.0822(13) |
| H16 | 0.362597 | −0.987868 | 0.241945 | 0.099* |
| C17 | 0.4446(7) | −1.0232(7) | 0.3374(3) | 0.0836(14) |
| H17 | 0.482987 | −1.120902 | 0.337195 | 0.100* |
| C18 | 0.3833(5) | −0.8065(6) | 0.3702(2) | 0.0632(10) |
| H18 | 0.369557 | −0.723831 | 0.396955 | 0.076* |

They often exhibit various coordination modes in metal coordination polymers. Some Cd(II)-based coordination complexes have been shown to be capable of binding with DNA, which might be potentially used for ablation of human bond cancer cells [7]. Based on the above considerations, in order to obtain the new metal coordination polymers, we selected bis(4-(1*H*-imidazol-1-yl)phenyl)amine as ligand for $Cd^{2+}$ coordination polymer $Cd(C_{18}N_5H_{15})_2(NO_3)_2$.

The asymmetric unit of **1** contains one half of a Cd(II) cation, one organic ligand and one $NO_3^-$. Within the structure, each $Cd^{2+}$ cation is six-coordinated with four N atoms from four different ligands and two oxygen atoms from two $NO_3^-$ anions, resulting in a $[CdN_4O_2]$ distorted octahedral geometry. The molecular structural unit is further assembled into a 2D structure. The bond lengths of Cd—N and Cd—O fall in their normal scopes and they are similar to those in known Cd(II)-coordination polymers [8, 9].

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