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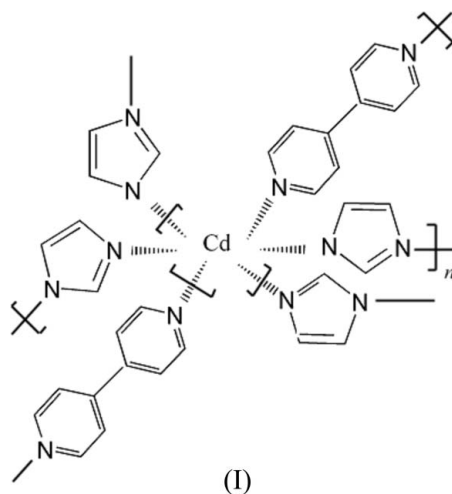
Key indicators

Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$
 R factor = 0.021
 wR factor = 0.055
Data-to-parameter ratio = 12.5For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Poly[μ_2 -4,4'-bipyridine-di- μ_2 -imidazolido-cadmium(II)]

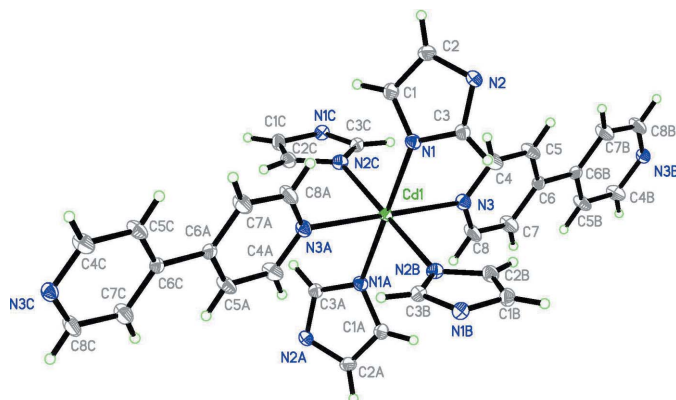
The title compound, $[\text{Cd}(\text{C}_{10}\text{H}_8\text{N}_2)(\text{C}_3\text{H}_4\text{N}_2)_2]_n$, is a new neutral centrosymmetric three-dimensional metal-organic framework structure. The metal atoms occupy inversion centres and the bipyridine ligands also possess C_i symmetry. The metal atoms are bridged by four imidazole ligands and two bipyridine units.

Comment

The construction of metal-organic frameworks (MOFs) is currently receiving considerable attention owing to their potential properties as functional solid materials, as well as their fascinating framework structures (Evans & Lin, 2002; Lu *et al.*, 2001; Li *et al.*, 1999). New materials spur new technologies (Snurr *et al.*, 2004), and these compounds can be potentially useful in gas storage, as molecular sieves, in size- and shape-selective catalysis, in magnetism, in optoelectronic devices, and so on (Eddaoudi *et al.*, 2002; Kitaura *et al.*, 2003; Moulton & Zaworotko, 2001; Millange *et al.*, 2002). These MOF structures can be rapidly, accurately and efficiently synthesized from relatively simple subunits, where the metal ions, multidentate organic ligands and coordinating bonds are the parameters for directing the self-assembly process. Our studies on the complexation of cadmium(II) salts with 4,4'-bipyridine (bpy) and imidazole has led to the formation of the title compound, (I), which has proved to have a polymeric centrosymmetric three-dimensional structure.

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A segment of the polymeric structure of compound (I) is illustrated in Fig. 1, and selected bond distances and angles are given in Table 1. The Cd^{II} atom lies on an inversion centre and the bipyridine ligand possesses C_i symmetry. The metal atoms


Figure 1

A view of part of the polymeric structure of compound (I), showing the atom-labelling scheme and with displacement ellipsoids drawn at the 50% probability level. [Symmetry codes: (A) $-x, -y, -z + 1$; (B) $x, -y + \frac{1}{2}, z - \frac{1}{2}$; (C) $-x, y - \frac{1}{2}, -z + \frac{3}{2}$]

are bridged by four imidazole ligands and two bipyridine units. The Cd–N_{imidazole} bond lengths vary from 2.324 (2) to 2.342 (2) Å and the Cd–N_{bipyridine} distances are 2.513 (2) Å. The *cis*-N–Cd–N bond angles range from 87.96 (7) to 92.04 (7)° (Table 1). The N atoms coordinate to the Cd^{II} centres in the monodentate mode (Fig. 1). On the basis of this connectivity, an interesting three-dimensional structure is built up, as shown in Fig. 2.

Experimental

Compound (I) was obtained by a hydrothermal reaction. The starting materials, Cd(OAc)₂·4H₂O (0.533 g, 2 mmol), imidazole (0.136 g, 2 mmol), 4,4'-bipyridine (0.1922 g, 1 mmol), and deionized water (15 ml) were mixed and the pH of the solution adjusted to 6.5 by the addition of sodium hydroxide (*ca* 0.08 g). The resulting suspension was stirred for 1 h, then sealed in a 40 ml stainless-steel bomb with a Teflon liner and heated at 458 K for 4 d. The autoclave was then cooled at 6 K h⁻¹ to 376 K. This temperature was maintained for 12 h, and then the system was cooled to room temperature at the same cooling rate. Colourless crystals of (I) were obtained and washed with water.

Crystal data

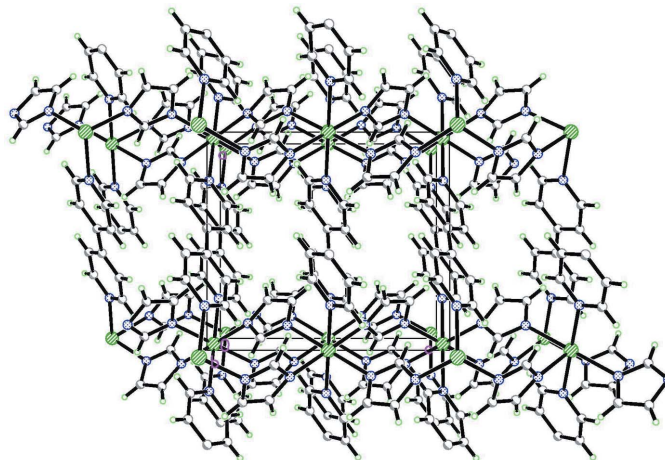
[Cd(C₁₀H₈N₂)(C₃H₄N₂)₂]
M_r = 402.73
 Monoclinic, *P*2₁/*c*
a = 9.2193 (13) Å
b = 7.9209 (12) Å
c = 10.2436 (15) Å
 β = 90.034 (2)°
V = 748.04 (19) Å³
Z = 2

D_x = 1.788 Mg m⁻³
 Mo *K*α radiation
 Cell parameters from 2578 reflections
 θ = 3.3–26.4°
 μ = 1.47 mm⁻¹
T = 293 (2) K
 Block, colourless
 0.20 × 0.18 × 0.10 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Bruker, 2000)
T_{min} = 0.560, *T_{max}* = 0.863
 3682 measured reflections

1323 independent reflections
 1150 reflections with *I* > 2σ(*I*)
R_{int} = 0.025
 θ_{\max} = 25.1°
h = -10 → 9
k = -7 → 9
l = -7 → 12


Figure 2

The polymeric network structure of compound (I), viewed along the *b* axis.

Refinement

Refinement on *F*²
R[*F*² > 2σ(*F*²)] = 0.021
wR(*F*²) = 0.055
S = 1.14
 1323 reflections
 106 parameters
 H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0205P)^2 + 0.5492P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.003$
 $\Delta\rho_{\max} = 0.26 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.67 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Cd1–N1	2.343 (2)	Cd1–N3	2.513 (2)
Cd1–N2 ⁱ	2.324 (2)		
N1 ⁱⁱ –Cd1–N1	180	N2 ⁱ –Cd1–N3 ⁱⁱⁱ	90.19 (7)
N2 ⁱ –Cd1–N2 ⁱⁱⁱ	180	N2 ⁱⁱⁱ –Cd1–N3 ⁱⁱ	89.81 (7)
N3 ⁱⁱ –Cd1–N3	180	N1 ⁱⁱⁱ –Cd1–N3 ⁱⁱ	89.25 (7)
N2 ⁱ –Cd1–N1 ⁱⁱ	87.96 (7)	N1–Cd1–N3 ⁱⁱ	90.75 (7)
N2 ⁱⁱⁱ –Cd1–N1 ⁱⁱ	92.04 (7)		

Symmetry codes: (i) $x, -y + \frac{1}{2}, z - \frac{1}{2}$; (ii) $-x, -y, -z + 1$; (iii) $-x, y - \frac{1}{2}, -z + \frac{3}{2}$

The H atoms were placed in calculated positions and constrained to ride on their parent atoms, with C–H distances of 0.93 Å and *U*_{iso}(H) = 1.2*U*_{eq}(C).

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Bruker, 2000); program(s) used to refine structure: SHELXTL; molecular graphics: PLATON (Spek, 2003); software used to prepare material for publication: SHELXTL.

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