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Key indicators

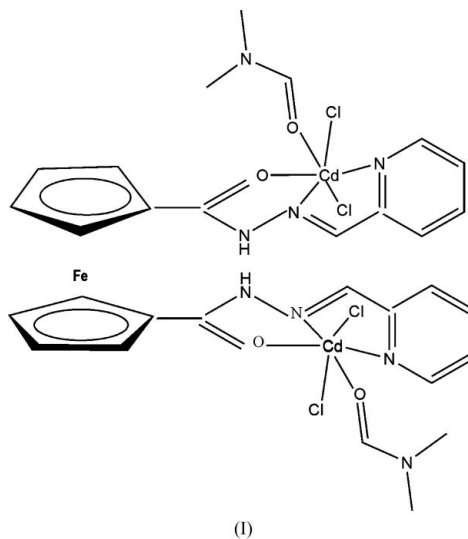
Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.008\text{ \AA}$
 R factor = 0.040
 wR factor = 0.072
Data-to-parameter ratio = 14.1For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**[μ -Bis(pyridine-2-carbaldehyde) (ferrocene-1,1'-diyl)dicarbonyl) dihydrazonato]bis-[dichloro(dimethylformamide)cadmium(II)]**

The title compound, $[\text{Cd}_2\text{Cl}_4\{\text{Fe}(\text{C}_{12}\text{H}_{10}\text{N}_3\text{O})_2\}(\text{C}_3\text{H}_7\text{NO})_2]$, has a twofold rotation axis passing through the Fe atom of the ferrocene spacer of the bis-tridentate ligand. The Cd^{II} atom is coordinated in a distorted octahedral geometry by carbonyl O, imine N and pyridine N atoms of the neutral bis-tridentate ligand, two chloride ions and an O atom from a dimethylformamide molecule. There are intramolecular $\text{N}-\text{H}\cdots\text{Cl}$ hydrogen bonds.

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Comment

The chemistry of ferrocene and its derivatives has attracted much interest, mainly because of their stability, good solubility and unusual reactivity and reversible redox properties (Togni & Hayashi, 1995). We have been interested in the preparation and the coordination chemistry of new multidentate ligands which contain two or three chelating arms linked to a ferrocene spacer (Guo *et al.*, 2002). The coordination behaviour of these ligands is characterized by a degree of variability in the structures of their complexes (Li *et al.*, 2004). Here we report the crystal structure of (I), which is a trinuclear complex with a bis-tridentate ligand (H_2L).



In (I), the Fe atom lies on a twofold rotation axis (Fig. 1), and the trinuclear complex consists of neutral ligand H_2L wrapped around two Cd^{II} atoms with four chloride anions as a charge balance. The Cd atom has a distorted octahedral geometry coordinated by a tridentate arm (O1/N2/N3), two chloride anions and a dimethylformamide (DMF) molecule (Table 1). The C6—O1 and C7—N2 bond distances are consistent with mostly double-bond character. In contrast, the

C6–N1 bond length is within the range for normal single bonds (Li *et al.*, 2006). The chloride anion Cl2 not only engages in the coordination but also forms an intramolecular N–H···Cl hydrogen bond (Table 2).

Experimental

All reagents were commercially available and of analytical grade. CdCl₂ (0.114 g, 0.35 mmol) was added to a solution of H₂L (0.084 g, 0.175 mmol) in DMF (3 ml). The solution was layered with Et₂O, and after 3 d, red crystals of (I) were obtained (yield 41%). Calculated for C₃₀H₃₄Cd₂Cl₄FeN₈O₄: C 36.25, H 3.42, N 11.28%; found: C 36.44, H 3.33, N 11.45%.

Crystal data

[Cd ₂ Fe(C ₁₂ H ₁₀ N ₃ O) ₂ Cl ₄ ·(C ₃ H ₇ NO) ₂]	<i>V</i> = 3591.0 (7) Å ³
<i>M_r</i> = 993.10	<i>Z</i> = 4
Monoclinic, <i>C2/c</i>	<i>D_x</i> = 1.837 Mg m ⁻³
<i>a</i> = 17.0582 (18) Å	Mo <i>K</i> α radiation
<i>b</i> = 16.9636 (18) Å	<i>μ</i> = 1.92 mm ⁻¹
<i>c</i> = 13.3243 (14) Å	<i>T</i> = 293 (2) K
<i>β</i> = 111.352 (2)°	Block, red
	0.20 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEX CCD diffractometer	3159 independent reflections
<i>ω</i> scans	2171 reflections with <i>I</i> > 2σ(<i>I</i>)
Absorption correction: none	<i>R</i> _{int} = 0.042
8838 measured reflections	<i>θ</i> _{max} = 25.0°

Refinement

Refinement on <i>F</i> ²	H-atom parameters constrained
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)] = 0.040	<i>w</i> = 1/[σ ² (<i>F</i> _o ²) + (0.018 <i>P</i>) ²]
<i>wR</i> [<i>F</i> ²] = 0.073	where <i>P</i> = (<i>F</i> _o ² + 2 <i>F</i> _c ²)/3
<i>S</i> = 1.02	(Δ/σ) _{max} = 0.001
3159 reflections	Δρ _{max} = 0.79 e Å ⁻³
224 parameters	Δρ _{min} = -0.44 e Å ⁻³

Table 1

Selected geometric parameters (Å, °).

Cd1–N2	2.314 (4)	Cd1–Cl2	2.5366 (12)
Cd1–N3	2.377 (4)	C6–O1	1.226 (6)
Cd1–Cl1	2.4103 (15)	C6–N1	1.356 (6)
Cd1–O1	2.416 (3)	C7–N2	1.275 (5)
Cd1–O2	2.466 (4)		
N2–Cd1–N3	68.75 (14)	Cl1–Cd1–O2	88.78 (11)
N2–Cd1–Cl1	166.71 (9)	O1–Cd1–O2	85.05 (12)
N3–Cd1–Cl1	112.68 (11)	N2–Cd1–Cl2	92.06 (9)
N2–Cd1–O1	66.93 (13)	N3–Cd1–Cl2	99.85 (9)
N3–Cd1–O1	135.43 (13)	Cl1–Cd1–Cl2	100.52 (5)
Cl1–Cd1–O1	109.35 (9)	O1–Cd1–Cl2	86.29 (8)
N2–Cd1–O2	78.28 (13)	O2–Cd1–Cl2	168.98 (10)
N3–Cd1–O2	81.72 (13)		

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
N1–H1A···Cl2 ⁱ	0.86	2.38	3.173 (4)	154

Symmetry code: (i) $-x, y, -z + \frac{3}{2}$.

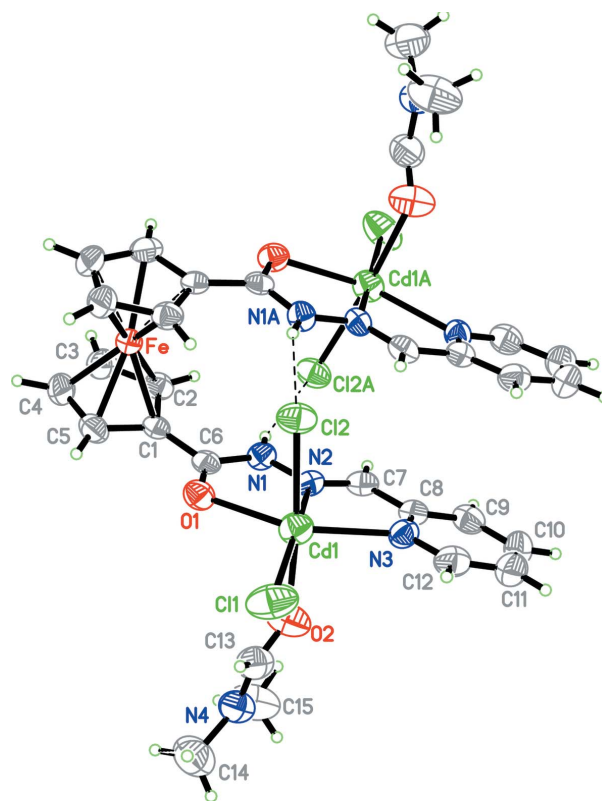


Figure 1

The molecular structure of (I), showing displacement ellipsoids drawn at the 50% probability level. Cd1A/N1A/Cl2A and unlabelled atoms are related to Cd1/N1/Cl2 and other labelled atoms by the symmetry operation $(-x, y, \frac{3}{2} - z)$. Dashed lines indicate hydrogen bonds.

All H atoms were positioned geometrically and refined as riding, with C–H = 0.93–0.98 Å, N–H = 0.86 Å, and *U*_{iso}(H) = 1.2*U*_{eq}(C,N) or 1.5*U*_{eq}(methyl C).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXL97*; software used to prepare material for publication: *SHELXL97*.

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