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Dichloridobis[3-(1*H*-imidazol-1-yl)-1-phenylpropan-1-one-κN^3]cadmium(II)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.028
wR factor = 0.056
Data-to-parameter ratio = 14.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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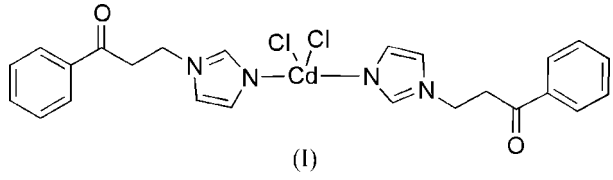
The molecular structure of the neutral title mononuclear complex, $[CdCl_2(C_{12}H_{12}N_2O)_2]$, is asymmetric, with the Cd^{II} atom located at the centre of a distorted tetrahedron. The Cd^{II} atom is coordinated by two N atoms of two distinct monodentate 3-(1*H*-imidazol-1-yl)-1-phenylpropan-1-one ligands and two Cl atoms. Intermolecular C—H···Cl and C—H···O hydrogen bonds link the monomeric units to produce a one-dimensional supramolecular chain in the [011] direction. These chains are further stabilized by intra-chain π–π stacking interactions between two neighbouring imidazole rings.

Comment

Aromatic ring stacking and hydrogen bonds are two important types of intramolecular non-covalent interactions, which play vital roles in highly efficient and specific biological reactions and are essential for molecular recognition and self-organization (Hunter, 1994; Borrows *et al.*, 1995). Very recently, we have described an Mn^{II}–*L*–NCS one-dimensional chain complex, $[ML_2(SCN)_2]_n$, [*L* is bis(3-(1*H*-imidazol-1-yl)-1-phenylpropan-1-one], in which significant stabilizing face-to-face π–π stacking interactions are observed (Cai *et al.*, 2007). In this contribution, we report the crystal structure of the title compound, $[CdCl_2(L)_2]$, (I), which is assembled into one-dimensional double chains *via* weak non-classical hydrogen bonds (C—H···Cl and C—H···O) and π–π stacking interactions.



(I)

The structure of the neutral mononuclear complex (I) is shown in Fig. 1, and selected bond lengths and angles are listed in Table 1. The coordination geometry of the Cd^{II} centre is distorted tetrahedral and comprises a pair of N atoms from two distinct *L* ligands and a pair of Cl atoms, with Cd—Cl distances of 2.4008 (8) and 2.4271 (8) Å, and Cd—N bond lengths of 2.220 (2) and 2.242 (2) Å. In this structure, there are two imidazole *L* ligands in the asymmetric unit, and the imidazole and phenyl rings in each of the ligands are not coplanar. The dihedral angles formed by the least-squares planes of the phenyl and imidazole rings are 77.00 (9) (C7–C12 and C1–C3,N1–N2) and 74.0 (1)° (C19–C24 and C13–C15, N3–N4).

Analysis of the crystal packing of (I) indicates that intermolecular C—H···Cl and C—H···O hydrogen bonds link the monomeric units to produce a one-dimensional supramolecular chain in the [011] direction, as shown in Fig. 2. The supramolecular structure of complex (I) is also stabilized by intra-chain π–π stacking interactions, with centroid-to-centroid distances between two neighbouring imidazole rings [at (x, y, z) and $(2-x, \frac{1}{2}+y, \frac{1}{2}-z)$] of 3.820 Å .

Experimental

$CdCl_2$ (18.2 mg, 0.1 mmol), bis(3-(1*H*-imidazol-1-yl)-1-phenylpropan-1-one (20.2 mg, 0.1 mmol) and NaN_3 (6.6 mg, 0.1 mmol) were mixed in a CH_3CN–H_2O (20 ml, 1:1 *v*/*v*) solution with vigorous stirring for *ca* 20 min. The resulting solution was filtered and left to stand at room temperature. Colourless prismatic crystals of (I) suitable for X-ray analysis were obtained in 55% yield by slow evaporation of the solvent over a period of 1.5 weeks. Analysis, calculated for $CdC_{24}H_{24}Cl_2N_4O_2$: C 49.38, H 4.14, N 9.60%; found: C 49.43, H 4.25, N 9.74%.

Crystal data

$[CdCl_2(C_{12}H_{12}N_2O)_2]$
M_r = 583.77
Monoclinic, $P2_1/c$
a = 9.2603 (13) Å
b = 9.2321 (13) Å
c = 28.902 (4) Å
β = 96.798 (2)°
V = 2453.5 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.14 mm^{-1}
T = 293 (2) K
0.30 × 0.14 × 0.12 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.606, T_{max} = 0.873
12625 measured reflections
4318 independent reflections
3554 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.056
S = 1.02
4318 reflections
298 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.56 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—N3	2.220 (2)	Cd1—Cl2	2.4008 (8)
Cd1—N1	2.242 (2)	Cd1—Cl1	2.4271 (8)
N3—Cd1—N1	101.04 (8)	N3—Cd1—Cl1	107.16 (6)
N3—Cd1—Cl2	117.06 (6)	N1—Cd1—Cl1	105.99 (6)
N1—Cd1—Cl2	111.71 (6)	Cl2—Cd1—Cl1	112.73 (3)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4*B*···Cl2^{i}	0.97	2.72	3.617 (3)	155
C5—H5*A*···O2^{ii}	0.97	2.48	3.316 (3)	145
C16—H16*A*···Cl1^{iii}	0.97	2.64	3.564 (3)	160

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

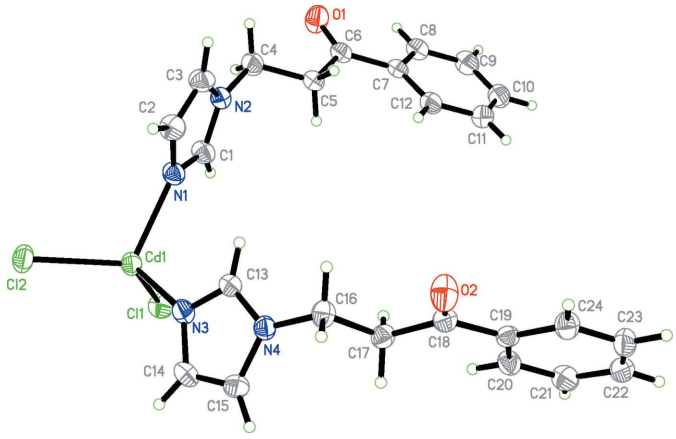


Figure 1
The molecular structure of the title complex, with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

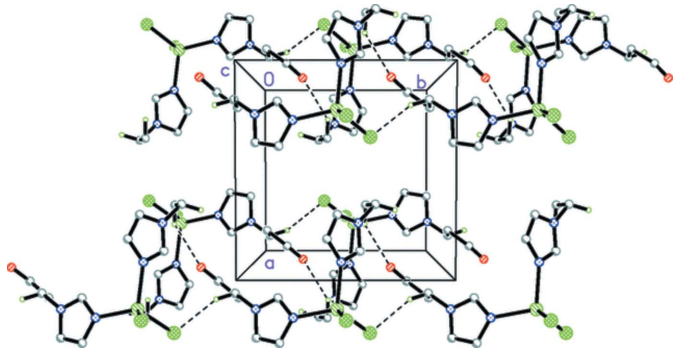


Figure 2
The one-dimensional supramolecular chain structure of the title complex, formed *via* C—H···Cl and C—H···O hydrogen-bonds (indicated by dashed lines). The *L* ligands have been partly omitted for clarity.

Although all H atoms were visible in a difference map, they were finally placed in geometrically calculated positions, with C—H distances in the range 0.93–0.97 Å, and included in the final refinement using the riding-model approximation, with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *APEX2* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

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