Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

{1-[(2-Chlorophenyl)diphenylmethyl]-1*H*-imidazole-κN^3}[tris(2-aminoethyl)amine-$\kappa^4 N$]-cadmium(II) bis(perchlorate)

Zhen-Ming Zhang,[a] Jian Gao,[b]* Tong-Tao Xu[b] and Da-Qi Wang[c]

[a]Department of Chemical Engineering, Huaihai Institute of Technology, Lianyungang 222005, People's Republic of China, [b]Department of Chemical Engineering, Lianyungang Technical College, Lianyungang 222006, People's Republic of China, and [c]College of Chemistry and Chemical Engineering, Liaocheng University, Shandong 252059, People's Republic of China

Correspondence e-mail: gaojian553@163.com

Received 22 October 2006
Accepted 3 November 2006

In the crystal structure of the title complex, $[Cd(C_{22}H_{17}ClN_2)(C_6H_{18}N_4)](ClO_4)_2$, the Cd^{II} atom is in a five-coordinate environment that exhibits a distorted trigonal–bipyramidal geometry.

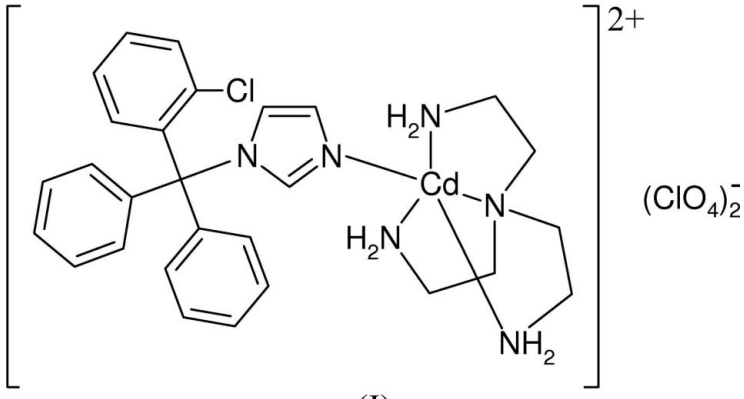
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.009 Å
Disorder in main residue
R factor = 0.048
wR factor = 0.122
Data-to-parameter ratio = 13.8

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

Comment

Clotrimazole, or 1-[(2-chlorophenyl)diphenylmethyl]-1*H*-imidazole ($C_{22}H_{17}ClN_2$), is an antifungal medication commonly used in the treatment of fungal infections of both humans and animals, such as vaginal yeast infections and ringworm. Coordination to metal ions of such an organic drug may lead to different biological activity (Navarro *et al.*, 2006). We report here the crystal structure of the title clotrimazole complex of Cd^{II}, (I).



(I)

The molecular structure of (I) is shown in Fig. 1. The Cd^{II} atom is in a five-coordinate environment; the value of the τ parameter (0.80) indicates that the geometry is close to trigonal bipyramidal (Addison *et al.*, 1984). Atoms N4, N5 and N6 comprise the equatorial plane, while atoms N1 and N3 lie in the axial positions. The Cd^{II} atom is displaced by 0.551 (1) Å from the equatorial plane, which forms a dihedral angle of 107.1 (1)° with the imidazole ring.

Experimental

A solution of tris(2-aminoethyl)amine (1.0 mmol) in 10 ml absolute methanol was added dropwise to a stirred solution of clotrimazole (1.0 mmol) and $Cd(ClO_4)_2{\cdot}6H_2O$ (1.0 mmol) in 30 ml absolute methanol. After stirring for 3 h at 320 K, the resulting precipitate was filtered off, washed with methanol and dried *in vacuo*. Single crystals of (I) were obtained by slow evaporation of the filtrate after 6 d.

Crystal data

$[Cd(C_{22}H_{17}ClN_2)(C_6H_{18}N_4)](ClO_4)_2$	V = 3327.6 (11) Å^3
M_r = 802.37	Z = 4
Monoclinic, $P2_1/c$	D_x = 1.602 Mg m^{-3}
a = 8.0031 (15) Å	Mo $K\alpha$ radiation
b = 22.004 (4) Å	μ = 0.95 mm^{-1}
c = 18.896 (4) Å	T = 298 (2) K
β = 90.406 (3)°	Block, yellow
	0.46 × 0.43 × 0.29 mm

Data collection

Bruker SMART 1000 CCD diffractometer	17363 measured reflections
	5875 independent reflections
φ and ω scans	4213 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	R_{int} = 0.037
	θ_{max} = 25.0°
T_{min} = 0.668, T_{max} = 0.769	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0436P)^2 + 7.6516P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.048	
$wR(F^2)$ = 0.122	
S = 1.02	$(\Delta/\sigma)_{max} < 0.001$
5875 reflections	$\Delta\rho_{max}$ = 0.79 e Å^{-3}
425 parameters	$\Delta\rho_{min}$ = −0.47 e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Cd1—N1	2.245 (4)	Cd1—N5	2.314 (4)
Cd1—N3	2.397 (4)	Cd1—N6	2.307 (5)
Cd1—N4	2.255 (5)		
N1—Cd1—N3	171.24 (15)	N3—Cd1—N5	75.70 (16)
N1—Cd1—N4	106.07 (17)	N3—Cd1—N6	75.24 (17)
N1—Cd1—N5	95.90 (16)	N4—Cd1—N5	123.29 (17)
N1—Cd1—N6	110.45 (17)	N4—Cd1—N6	110.58 (18)
N3—Cd1—N4	77.19 (17)	N5—Cd1—N6	109.14 (19)

H atoms were positioned geometrically and allowed to ride on their parent atoms, with aromatic C—H = 0.93 Å, primary amine N—H = 0.90 Å and methylene C—H = 0.97 Å. The U_{iso}(H) values were set at 1.2U_{eq}(C) for all H atoms. The Cl atom of the cation was found to be disordered. The site-occupancy factors of atoms Cl1 and Cl1′ were constrained to sum to unity, and refined to 0.664 (4) and 0.336 (4), respectively. Restraints were applied to the displacement parameters of the perchlorate anions, and the displacement parameters of the O atoms were restrained to approximate isotropic behaviour.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); 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, 1997); software used to prepare material for publication: *SHELXTL*.

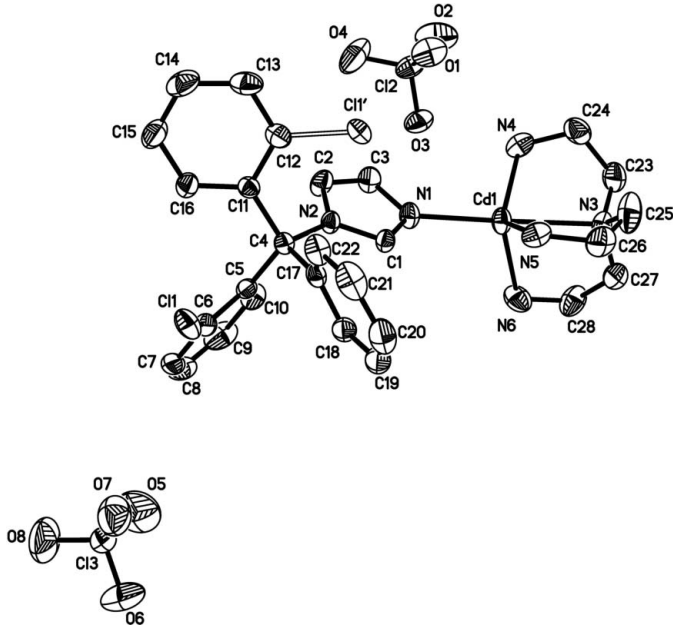


Figure 1
The molecular structure of (I), showing displacement ellipsoids drawn at the 30% probability level. H atoms have been omitted. Atoms Cl1 and Cl1′ have site-occupancy factors of 0.664 (4) and 0.336 (4), respectively.

This work was supported by the Key Laboratory of Marine Biotechnology of Jiangsu Province.

References

Addison, A. W., Rao, T. N., Reedijk, J., van Rijn, J. & Verschoor, G. C. (1984). *J. Chem. Soc. Dalton Trans.* pp. 1349–1356.
Bruker (1997). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Navarro, M., Pena, N. P., Colmenares, I., Gonzalez, T., Arsenak, M. & Taylor, P. (2006). *J. Inorg. Biochem.* **100**, 152–157.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Siemens (1996). *SMART* and *SAINT*. Versions 4.0. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.