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

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.008 Å
R factor = 0.056
wR factor = 0.165
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.

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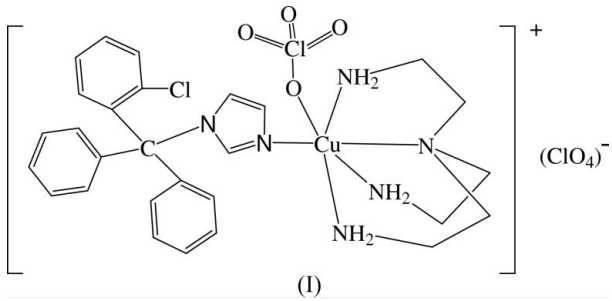
In the crystal structure of the title compound, $[Cu(ClO_4)(C_{22}H_{17}ClN_2)(C_6H_{18}N_4)]ClO_4$, the Cu^{II} ion assumes a distorted octahedral coordination geometry.

Comment

Clotrimazole {or 1-[(2-chlorophenyl)diphenylmethyl]-1*H*-imidazole}, is an imidazole *N*-substituted antifungal agent commonly used in the treatment of fungal infections of both humans and animals such as vaginal yeast infections and ringworm. The coordination of such an organic drug with known biological activities to a metal may produce different biological activity (Navarro et al., 2006). We report here the crystal structure of the title clotrimazole complex of Cu^{II}, (I).



(I)

The molecular structure of (I) is shown in Fig. 1. The Cu^{II} ion is located in an N_5O coordination environment with a distorted octahedral geometry. Atoms N4, N5, N6 and O1 form the equatorial plane, with a maximum deviation of 0.093 (2) Å for O1. Atoms N2 and N3 occupy the axial positions, with an N2—Cu1—N3 bond angle of 177.12 (15)° (Table 1). The Cu^{II} ion is displaced by 0.168 (2) Å from the equatorial plane.

N—H···O hydrogen bonding between amino and perchlorate groups (Table 2) helps to stabilize the crystal structure.

Experimental

To a stirred solution of clotrimazole (1.0 mmol) and $Cu(ClO_4)_2\cdot 6H_2O$ (1.0 mmol) in absolute methanol (30 ml), a solution of tris(2-aminoethyl)amine (1.0 mmol) in absolute methanol (10 ml) was added dropwise. After stirring for 2 h at 320 K, the resulting precipitate was filtered off. Single crystals of (I) were obtained by slow evaporation of the filtrate after 16 d.

Crystal data

$[Cu(ClO_4)(C_{22}H_{17}ClN_2)(C_6H_{18}N_4)]$-$ClO_4$	V = 3200.2 (12) Å^3
M_r = 753.51	Z = 4
Monoclinic, $P2_1/c$	D_x = 1.564 Mg m^{-3}
a = 7.7303 (16) Å	Mo $K\alpha$ radiation
b = 21.938 (5) Å	μ = 0.99 mm^{-1}
c = 18.932 (4) Å	T = 298 (2) K
β = 94.614 (3)°	Block, blue
	0.40 × 0.29 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer	16722 measured reflections
φ and ω scans	5760 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)	4006 reflections with $I > 2\sigma(I)$
T_{min} = 0.692, T_{max} = 0.826	R_{int} = 0.037
	θ_{max} = 25.2°

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0787P)^2 + 6.2079P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.056	$(\Delta/\sigma)_{max}$ = 0.001
$wR(F^2)$ = 0.165	$\Delta\rho_{max}$ = 0.98 e Å^{-3}
S = 1.02	$\Delta\rho_{min}$ = −0.53 e Å^{-3}
5760 reflections	
416 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	2.453 (4)	Cu1—N4	2.095 (4)
Cu1—N2	2.066 (3)	Cu1—N5	2.075 (4)
Cu1—N3	2.104 (4)	Cu1—N6	2.077 (4)
N2—Cu1—N5	97.48 (15)	N6—Cu1—N3	83.79 (15)
N2—Cu1—N6	98.58 (15)	N4—Cu1—N3	83.31 (15)
N5—Cu1—N6	97.78 (17)	N2—Cu1—O1	86.43 (13)
N2—Cu1—N4	93.93 (14)	N5—Cu1—O1	174.20 (15)
N5—Cu1—N4	98.53 (16)	N6—Cu1—O1	85.81 (14)
N6—Cu1—N4	157.93 (15)	N4—Cu1—O1	76.87 (13)
N2—Cu1—N3	177.12 (15)	N3—Cu1—O1	92.15 (15)
N5—Cu1—N3	83.76 (16)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4A···O2^{i}	0.90	2.34	3.172 (6)	154
N4—H4B···O4^{ii}	0.90	2.35	3.127 (7)	144
N5—H5A···O8	0.90	2.21	3.068 (7)	160
N5—H5B···O3^{i}	0.90	2.14	3.030 (6)	171
N6—H6A···O3	0.90	2.28	3.074 (6)	147
N6—H6B···O7	0.90	2.33	3.222 (8)	174

Symmetry codes: (i) $x-1, y, z$; (ii) $-x+2, -y+1, -z+1$.

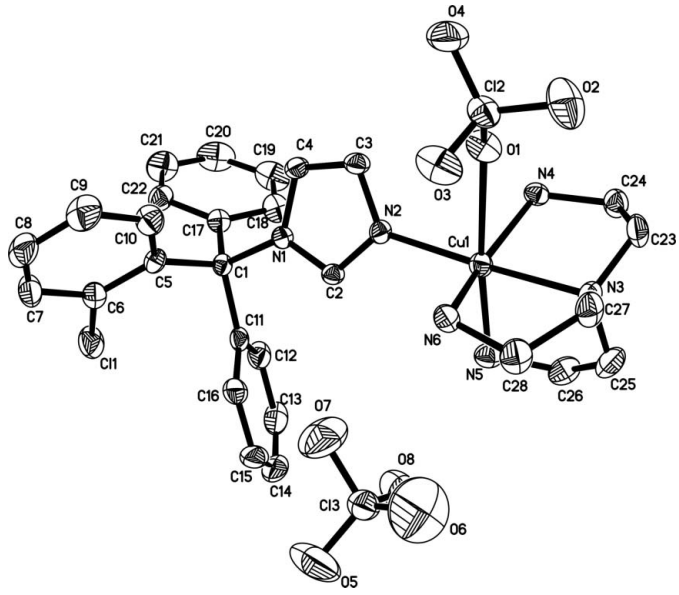


Figure 1
The molecular structure of (I), shown with 30% probability displacement ellipsoids. H atoms have been omitted for clarity.

H atoms were positioned geometrically and treated as riding 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. U_{iso}(H) values were set at $1.2U_{eq}$(C,N).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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