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Key indicators

Single-crystal X-ray study
 T = 298 K
 Mean $\sigma(C-C)$ = 0.010 Å
 R factor = 0.049
 wR factor = 0.134
 Data-to-parameter ratio = 13.7

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

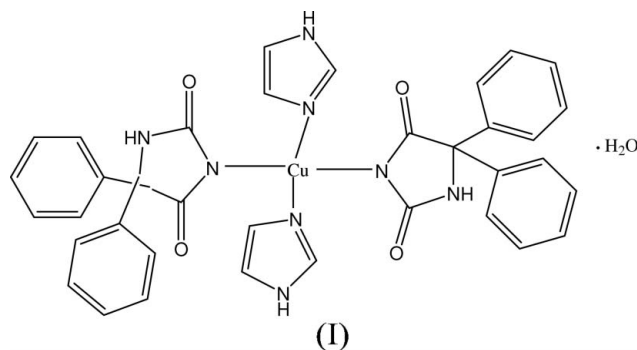
Bis(5,5-diphenylhydantoinato- κN^3)bis(1H-imidazole- κN^3)copper(II) monohydrate

In the title compound, $[Cu(C_{15}H_{11}N_2O_2)_2(C_3H_4N_2)_2] \cdot H_2O$, the Cu^{II} ion has a distorted square-planar CuN₄ coordination environment. The crystal structure is stabilized by intermolecular hydrogen bonding.

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Comment

As part of an ongoing investigation of Cu^{II} complexes, we report here the structure of the title Cu^{II} complex, (I).



The molecular structure of (I) is shown in Fig. 1. The Cu^{II} ion has a distorted square-planar CuN₄ coordination geometry, formed by two 5,5-diphenylhydantoin and two imidazole ligands. The N5—Cu1—N7 bond angle of 166.2 (3)° indicates the degree of distortion (Table 1). The dihedral angle between the imidazole rings is 87.0 (6)°.

The solvent water molecule links with the complex molecule via O—H...O hydrogen bonding, and intermolecular N—H...O hydrogen bonding occurs between neighbouring complex molecules (Table 2); these interactions stabilize the crystal structure of (I).

Experimental

To a stirred methanol solution (20 ml) of 5,5-diphenylhydantoin (1 mmol) and Cu(CH₃COO)₂·2H₂O (1 mmol) was added dropwise a methanol solution (10 ml) of imidazole (1.0 mmol) at room temperature. After stirring for 3 h at 320 K, the solution was filtered. Single crystals of (I) were obtained from the filtrate after 10 d.

Crystal data

$[Cu(C_{15}H_{11}N_2O_2)_2(C_3H_4N_2)_2] \cdot H_2O$	Z = 4
$M_r = 720.24$	$D_x = 1.357 \text{ Mg m}^{-3}$
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation
$a = 8.615 (2) \text{ \AA}$	$\mu = 0.67 \text{ mm}^{-1}$
$b = 16.576 (3) \text{ \AA}$	T = 298 (2) K
$c = 24.680 (4) \text{ \AA}$	Prism, red
$V = 3524.4 (12) \text{ \AA}^3$	0.38 × 0.21 × 0.11 mm

Data collection

Bruker APEX area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 2002)
 $T_{\min} = 0.784$, $T_{\max} = 0.930$

18479 measured reflections
 6182 independent reflections
 3915 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.061$
 $\theta_{\text{max}} = 25.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.049$
 $wR(F^2) = 0.134$
 $S = 0.97$
 6182 reflections
 451 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0594P)^2 + 1.5734P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.53 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.38 \text{ e } \text{\AA}^{-3}$
 Absolute structure: Flack (1983),
 2664 Friedel pairs
 Flack parameter: 0.52 (2)

Table 1

Selected geometric parameters (\AA , $^\circ$).

Cu1—N1	1.974 (4)	Cu1—N5	1.971 (5)
Cu1—N3	1.969 (4)	Cu1—N7	1.990 (5)
N3—Cu1—N5	91.10 (17)	N3—Cu1—N7	87.41 (18)
N3—Cu1—N1	174.78 (17)	N5—Cu1—N7	166.2 (2)
N5—Cu1—N1	93.71 (18)	N1—Cu1—N7	88.40 (19)

Table 2

Hydrogen-bond geometry (\AA , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2—H2 \cdots O4 ⁱ	0.86	2.13	2.950 (5)	158
N4—H4 \cdots O2 ⁱⁱ	0.86	2.02	2.827 (5)	156
N6—H6 \cdots O3 ⁱⁱⁱ	0.86	1.88	2.720 (7)	164
N8—H8 \cdots O5 ^{iv}	0.86	1.94	2.787 (7)	167
O5—H1 \cdots O4	0.85	1.90	2.714 (6)	160
O5—H3 \cdots O2	0.85	1.89	2.665 (6)	152

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

H atoms were positioned geometrically, with C—H = 0.93 and N—H = 0.86 \AA , and refined in riding mode, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$.

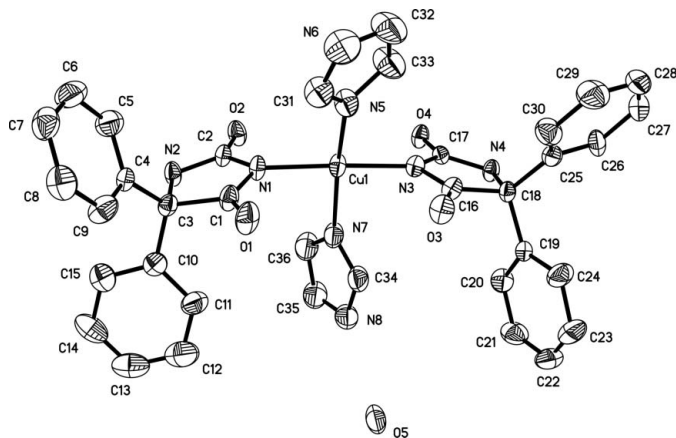


Figure 1

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

solvent-accessible void of 46\AA^3 was found in the final difference Fourier map but no solvent molecule could be located there.

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

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References

- Bruker (2003). SAINT (Version 6.45a) and SMART (Version 5.059). Bruker AXS Inc., Madison, Wisconsin, USA.
 Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.
 Sheldrick, G. M. (1997a). SHELXS97 and SHELXL97. University Göttingen, Germany.
 Sheldrick, G. M. (1997b). SHELXTL. Version 5.10. Bruker AXS, Inc., Madison, Wisconsin, USA.
 Sheldrick, G. M. (2002). SADABS. Version 2.03. University of Göttingen, Germany.