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trans-Diaquabis(5,5-diphenylhydantoinato-κN^3)-copper(II)

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.007 Å
R factor = 0.050
wR factor = 0.136
Data-to-parameter ratio = 13.6

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

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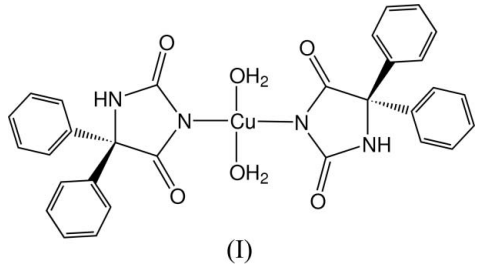
The molecule of the title complex, $[Cu(C_{15}H_{11}N_2O_2)_2(H_2O)_2]$, lies on a twofold rotation axis. The crystal structure is based on a network of intermolecular N—H···O=C and O—H···O=C interactions.

Comment

5,5-Diphenylimidazoline-2,4-dione, also known as phenytoin or PHT, is a widely used drug in the treatment of epilepsy. However, 5,5-diphenylimidazoline-2,4-dione possesses toxicological properties which limit its usefulness. So a thorough analysis of its complex structure will be very helpful. We report here the synthesis and crystal structure of a copper(II) complex of PHT.

From Fig. 1, it can be seen that the title compound, $[Cu(pht)_2(H_2O)_2]$, (I), is a molecular complex (pht is the 5,5-diphenylhydantoinate anion, derived from diphenylhydantoin, *i.e.* 5,5-diphenyl-2,4-imidazolidinedione). The Cu atom lies on a twofold rotation axis and is *trans*-coordinated by two N atoms from two pht ligands and two water molecules. The water molecules also lie on the twofold axis.



(I)

Bond lengths and angles around the Cu atom (Table 1) show that the metal centre has an almost ideal square-planar geometry, with a dihedral angle of 49.5 (1)° between the planes of atoms N1/C1/N2/C3/C2 and O3/O4/N1/N1^{i} [symmetry code: (i) $1-x, y, -z+\frac{1}{2}$]. The dihedral angles between the pht plane and the planes of the phenyl rings are 63.3 (2) (phenyl ring C4–C9) and 65.1 (2)° (phenyl ring C10–C15). The phenyl rings make a dihedral angle of 87.1 (2)°.

From Fig. 2 it can be seen that the complex forms a network structure assembled by intermolecular N—H···O=C and O—H···O=C hydrogen bonds, involving carbonyl and amine functionalities of adjacent pht groups and water molecules (Table 2).

Experimental

To a solution of 5,5-diphenyl-2,4-imidazolidine dione (1 mmol) in methanol (10 ml) were added copper(II) acetate monohydrate

(0.5 mmol) and a solution of tris(3-aminopropyl)amine (1 mmol) in methanol (10 ml). The reaction mixture was stirred for 30 h at 429 K. Violet–red prismatic crystals of (I) were obtained after cooling the reaction to 298 K (m.p. 508 K). Analysis, calculated for $C_{30}H_{26}N_4O_6Cu$: C 59.84, H 4.35, N 13.96%; found: C 59.46, H 4.21, N 13.68%.

Crystal data

$[Cu(C_{15}H_{11}N_2O_2)_2(H_2O)_2]$	$Z = 4$
$M_r = 602.09$	$D_x = 1.383$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
$a = 31.341$ (7) Å	$\mu = 0.80$ mm^{-1}
$b = 8.5690$ (19) Å	$T = 298$ (2) K
$c = 11.287$ (3) Å	Block, violet-red
$\beta = 107.411$ (4)°	0.33 × 0.15 × 0.05 mm
$V = 2892.4$ (11) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	7319 measured reflections
	2544 independent reflections
φ and ω scans	1861 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.039$
	$\theta_{max} = 25.0°$
$T_{min} = 0.777$, $T_{max} = 0.961$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.078P)^2 + 1.2445P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.050$	
$wR(F^2) = 0.136$	
$S = 1.02$	$(\Delta/\sigma)_{max} < 0.001$
2544 reflections	$\Delta\rho_{max} = 0.36$ e Å^{-3}
187 parameters	$\Delta\rho_{min} = -0.44$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	1.991 (3)	Cu1—O4	2.006 (4)
Cu1—O3	1.982 (5)		
N1—Cu1—O3	90.28 (8)	N1^i—Cu1—N1	179.44 (16)
N1—Cu1—O4	89.72 (8)	O3—Cu1—O4	180

Symmetry code: (i) $-x+1, y, -z+\frac{1}{2}$.

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O1^{ii}	0.86	2.02	2.878 (4)	177
O3—H16···O2^i	0.85	2.49	2.918 (3)	112
O4—H17···O2^{iii}	0.85	2.27	2.902 (2)	132

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

All H atoms were positioned geometrically and treated as riding on their parent atoms, with restrained distances as follows: aromatic C—H = 0.93 Å, amine N–H = 0.86 Å and water O—H = 0.85 Å. Isotropic displacement parameters for H atoms were fixed at $U_{iso}(H) = 1.2U_{eq}$(carrier atom).

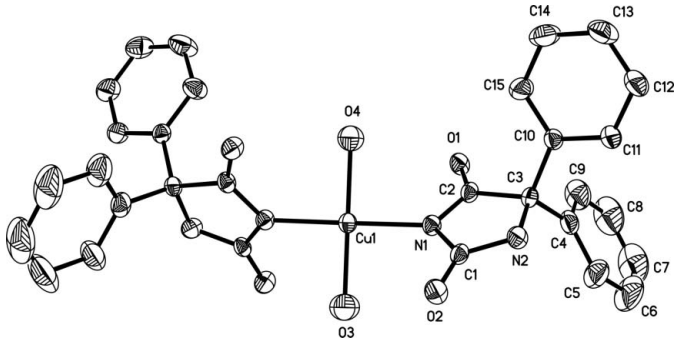


Figure 1
The structure of the title complex, with displacement ellipsoids at the 30% probability level and the labelling scheme for the asymmetric unit. Non-labelled atoms are generated by symmetry operator $(1-x, y, \frac{1}{2}-z)$. H atoms have been omitted for clarity.

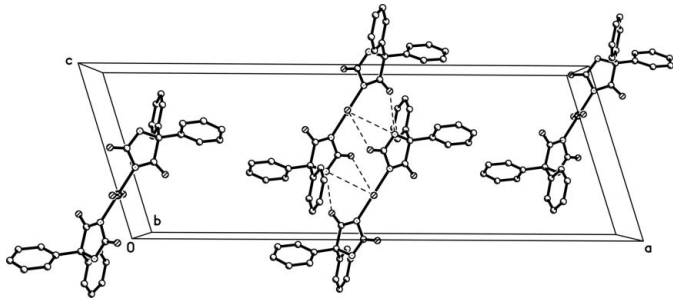


Figure 2
The crystal packing of the title complex, viewed down the [010] axis. Dashed lines represent hydrogen-bonding contacts. H atoms have been omitted for clarity.

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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