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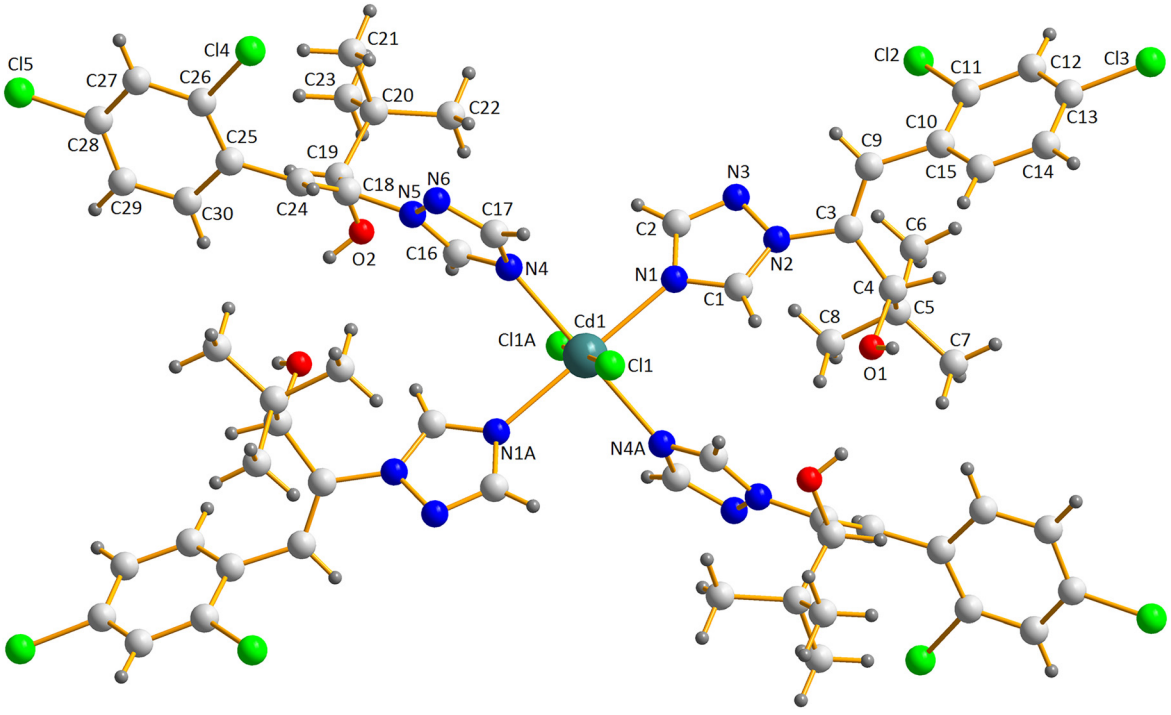
Crystal structure of dichlorido-tetrakis((*E*)-(*RS*)-1-(2,4-dichlorophenyl)-4,4-dimethyl-2-(1,2,4-triazol-1-yl)pent-1-en-3-ol-κ^1N)cadmium(II), $C_{60}H_{68}O_4N_{12}Cl_{10}Cd$



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Abstract

$C_{60}H_{68}O_4N_{12}Cl_{10}Cd$, triclinic, $P\bar{1}$ (no. 2), a = 8.9686(15) Å, b = 13.554(2) Å, c = 15.365(3) Å, α = 92.113(3)°, β = 99.047(3)°, γ = 106.492(3)°, V = 1762.1(5) Å^3, Z = 1, $R_{gt}(F)$ = 0.0436, $wR_{ref}(F^2)$ = 0.1130, T = 296(2) K.

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Table 1: Data collection and handling.

Crystal:	Colourless rodlike
Size	0.38 × 0.27 × 0.14 mm
Wavelength:	Mo *Kα* radiation (0.71073 Å)
μ:	0.74 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max}, completeness:	25.4°, 98%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	9011, 6347, 0.024
Criterion for I_{obs}, $N(hkl)_{gt}$:	I_{obs} > 2 σ(I_{obs}), 5112
$N(param)_{refined}$:	402
Programs:	Bruker [1], SHELX [2–4], Diamond [5]

The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	U_{iso}^*/U_{eq}
C1	−0.1848 (4)	0.0788 (3)	0.6469 (2)	0.0426 (9)
H1	−0.281390	0.033638	0.619901	0.051*
C2	0.0505 (5)	0.1665 (3)	0.6764 (3)	0.0594 (11)
H2	0.156000	0.194307	0.671532	0.071*
C3	−0.2730 (4)	0.1417 (3)	0.7790 (2)	0.0350 (8)
C4	−0.3702 (4)	0.0414 (3)	0.8052 (2)	0.0404 (8)
H4	−0.454707	0.055959	0.832026	0.048*
C5	−0.2809 (5)	−0.0133 (3)	0.8728 (2)	0.0581 (11)
C6	−0.1923 (7)	0.0642 (4)	0.9510 (3)	0.0901 (17)
H6A	−0.148269	0.029440	0.997029	0.135*
H6B	−0.263750	0.095952	0.972798	0.135*
H6C	−0.108830	0.116321	0.932416	0.135*
C7	−0.4035 (7)	−0.1011 (4)	0.9039 (3)	0.0884 (16)
H7A	−0.459655	−0.149940	0.854488	0.133*
H7B	−0.476430	−0.073914	0.929206	0.133*
H7C	−0.351662	−0.134878	0.947616	0.133*
C8	−0.1655 (6)	−0.0578 (4)	0.8316 (3)	0.0823 (15)
H8A	−0.078406	−0.002225	0.820726	0.123*
H8B	−0.219174	−0.097468	0.776857	0.123*
H8C	−0.126911	−0.101352	0.871586	0.123*
C9	−0.2722 (4)	0.2353 (3)	0.8062 (2)	0.0404 (8)
H9	−0.198667	0.290547	0.788161	0.049*
C10	−0.3782 (4)	0.2606 (3)	0.8631 (2)	0.0388 (8)
C11	−0.3159 (5)	0.3202 (3)	0.9427 (2)	0.0470 (9)
C12	−0.4116 (6)	0.3505 (3)	0.9944 (3)	0.0599 (11)
H12	−0.368273	0.389870	1.048123	0.072*
C13	−0.5701 (6)	0.3214 (3)	0.9648 (3)	0.0565 (11)
C14	−0.6371 (5)	0.2604 (3)	0.8871 (3)	0.0595 (11)
H14	−0.746127	0.239099	0.868814	0.071*
C15	−0.5395 (5)	0.2315 (3)	0.8366 (2)	0.0492 (10)
H15	−0.583929	0.191417	0.783347	0.059*
C16	0.3162 (4)	0.1650 (3)	0.4569 (2)	0.0409 (8)
H16	0.378303	0.130027	0.489499	0.049*
C17	0.1280 (5)	0.2161 (3)	0.4011 (3)	0.0593 (11)
H17	0.026170	0.221812	0.387796	0.071*
C18	0.5233 (4)	0.2780 (2)	0.3822 (2)	0.0342 (7)
C19	0.6609 (4)	0.2798 (3)	0.4531 (2)	0.0381 (8)
H19	0.754299	0.292668	0.424703	0.046*
C20	0.6990 (5)	0.3650 (3)	0.5301 (2)	0.0487 (9)
C21	0.7133 (6)	0.4682 (3)	0.4915 (3)	0.0795 (15)
H21A	0.612887	0.467697	0.458331	0.119*
H21B	0.790263	0.479713	0.453115	0.119*
H21C	0.745745	0.522536	0.538499	0.119*
C22	0.5774 (5)	0.3462 (4)	0.5914 (3)	0.0724 (13)
H22A	0.612394	0.398446	0.640068	0.109*
H22B	0.565442	0.279467	0.613362	0.109*
H22C	0.477883	0.348655	0.559251	0.109*
C23	0.8588 (5)	0.3672 (4)	0.5840 (3)	0.0798 (14)
H23A	0.938021	0.383304	0.547063	0.120*
H23B	0.852120	0.300768	0.605627	0.120*
H23C	0.886605	0.418727	0.633012	0.120*
C24	0.5334 (4)	0.3122 (3)	0.3034 (2)	0.0421 (8)
H24	0.440482	0.312837	0.267037	0.051*
C25	0.6833 (4)	0.3497 (3)	0.2693 (2)	0.0399 (8)
C26	0.7364 (4)	0.4498 (3)	0.2446 (2)	0.0434 (9)
C27	0.8800 (4)	0.4869 (3)	0.2168 (2)	0.0460 (9)
H27	0.913840	0.554450	0.201569	0.055*
C28	0.9716 (4)	0.4215 (3)	0.2122 (2)	0.0446 (9)
C29	0.9183 (5)	0.3197 (3)	0.2304 (2)	0.0510 (10)
H29	0.978282	0.274990	0.223835	0.061*
C30	0.7745 (5)	0.2851 (3)	0.2584 (2)	0.0501 (9)
H30	0.738417	0.216361	0.270221	0.060*
Cd1	0.000000	0.000000	0.500000	0.03324 (12)
Cl1	−0.24504 (11)	0.01937 (8)	0.38873 (6)	0.0543 (3)
Cl2	−0.11412 (14)	0.35692 (9)	0.98031 (7)	0.0738 (3)
Cl3	−0.68996 (19)	0.35993 (11)	1.02901 (10)	0.1017 (5)
Cl4	0.62325 (14)	0.53375 (9)	0.25159 (8)	0.0729 (4)
Cl5	1.15735 (12)	0.46744 (9)	0.18471 (7)	0.0674 (3)
N1	−0.0523 (3)	0.0953 (2)	0.61522 (18)	0.0450 (7)
N2	−0.1610 (3)	0.1356 (2)	0.72270 (17)	0.0388 (7)
N3	−0.0074 (4)	0.1937 (3)	0.7426 (2)	0.0583 (9)
N4	0.1646 (3)	0.1481 (2)	0.45533 (19)	0.0436 (7)
N5	0.3691 (3)	0.2396 (2)	0.40494 (18)	0.0364 (6)
N6	0.2466 (4)	0.2743 (3)	0.3680 (2)	0.0562 (9)
O1	−0.4439 (3)	−0.0306 (2)	0.72917 (17)	0.0512 (7)
H1A	−0.529751	−0.022905	0.709118	0.077*
O2	0.6416 (3)	0.18272 (19)	0.48937 (16)	0.0489 (6)
H2A	0.662272	0.142582	0.455209	0.073*

Source of material

The (*E*)-(*RS*)-1-(2,4-dichlorophenyl)-4,4-dimethyl-2- (1,2,4-triazol-1-yl)pent-1-en-3-ol (0.653 g, 0.200 mmol) was dissolved in propanone (10 mL). Then, cadmium chloride 2.5 hydrate (0.114 g, 0.050 mmol) was added. The reaction mixture was allowed to stir at room temperature for 2 h. Colorless rod-shaped crystals of the title compound were obtained by slow evaporation from propanone. **Anal. Calcd.** (%) for $[Cd(L_2)Cl_2]$. C, 48.43; H, 4.61; N, 11.29; found (%): C, 48.40; H, 4.59; N, 11.35.

Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms, with C–H = 0.96 Å (methyl), U_{iso}(H) = 1.5 U_{eq}(C), C–H = 0.98 Å (methine), U_{iso}(H) = 1.2 U_{eq}(C), C–H = 0.93 Å (aromatic and alkenyl), U_{iso}(H) = 1.2 U_{eq}(C), and O–H = 0.82 Å (hydroxyl), U_{iso}(H) = 1.5 U_{eq}(O).

Comment

Pesticides are widely used in agricultural production to control molds, pests, weeds and therefore ensure high quality and high yields of vegetables, fruits and crops all over the world [6, 7]. Triazole fungicides have the advantages of high efficiency, broad spectrum, low toxicity to nontarget organisms, and low resistance [8]. Triazole fungicides which inhibit the biosynthesis of fungal ergosterol, can be used to control fungal diseases, such as powdery mildews, rusts, and many leaf spot fungi on a variety of plants [9, 10].

Diniconazole, systematic name: (*E*)-(*RS*)-1-(2,4-dichlorophenyl)-4,4-dimethyl-2-(1H-1,2,4-triazol-1-yl) pent-1-en-3-ol is a systemic fungicide showing fungitoxicity to a broad range of fungal species [11]. Its known to inhibit the biosynthesis of ergo sterol in fungal species [12]. The pharmacological and toxicological properties of many drugs are improved when they form metal complexes [13–14]. In this paper, a new diniconazole Cd(II) complex is described.

The title compound contains a mononuclear complex. The asymmetric unit is half of the title complex. As is shown in the figure, the Cd(II) cation is six-coordinated by two chlorido ligands and four N atoms from four diniconazole ligands in a distorted regular octahedral environment. The Cd–N length (Cd1–N1 = 2.336(3) Å, Cd1–N4 = 2.328(3) Å) and Cd–Cl length (Cd1–Cl1 = 2.646(1) Å), the N1–Cd1–N4, N1–Cd1–$N4^{i}$, N1–Cd1–Cl1, N4–Cd1–Cl1, N1–Cd1–$Cl1^{i}$, and N4–Cd1–$Cl1^{i}$ bond angles of 91.58(10)°, 88.42(10)°, 92.48(7)°, 91.01(8)°, 87.52(7)°, and 88.99(8)°, respectively (symmetry code: (i) $-x, -y, -z+1$) are all in the expected ranges. The Cd(II) is located on the center of symmetry of the title compound, so each bond angle of N1–Cd1–$N1^{ii}$, N4–Cd1–$N4^{ii}$, and Cl1–Cd–$Cl1^{ii}$ is 180°. These are in agreement with closely related Cd(II) complexes reported. The title structure contains hydrogen bonds O1–H1A$\cdots$$Cl1^{ii}$ ($d_{O1\cdots Cl1}$ = 3.124(3) Å, 162.0°, symmetry code: (ii) $-x-1, -y, -z+1$) and O2–H2A$\cdots$$Cl1^{iV}$ ($d_{O2\cdots Cl1}$ = 3.138(3) Å, 166.3°, symmetry code: (iii) $x+1, y, z$) forming a one-dimensional (1D) chain along the a-axis.

Author contributions: All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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