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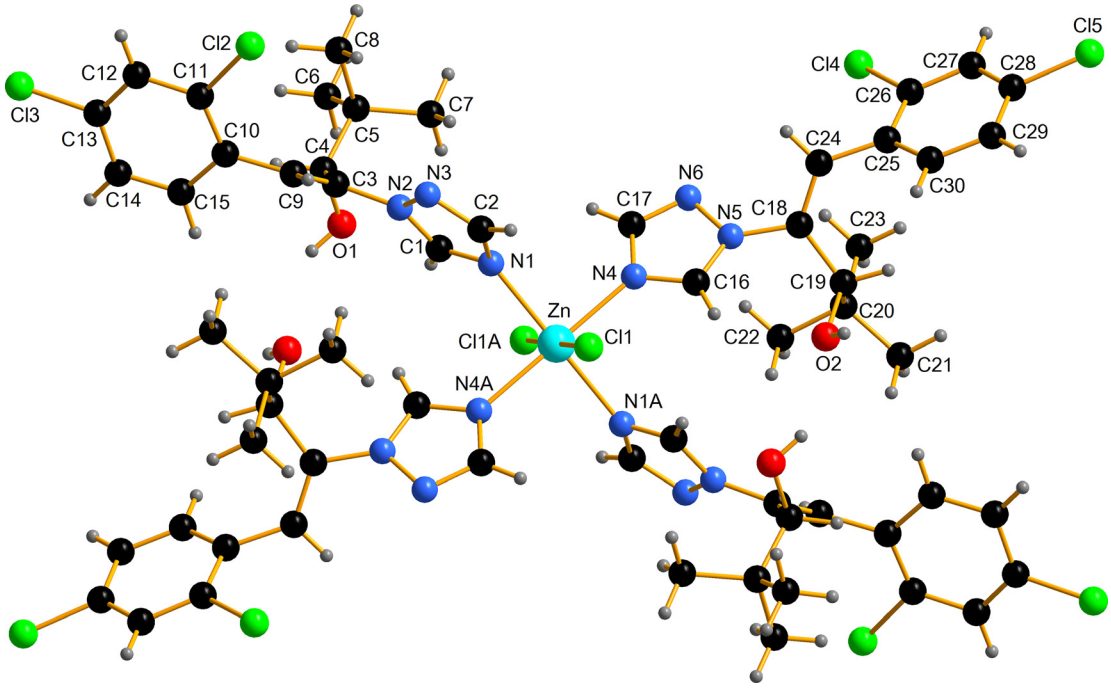
Crystal structure of dichlorido-tetra((*E*)-(*RS*)-1-(2,4-dichlorophenyl)-4,4-dimethyl-2-(1,2,4-triazol-1-yl)pent-1-en-3-ol-κ^1*N*)zinc(II), $C_{60}H_{68}O_4N_{12}Cl_{10}Zn$



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Abstract

$C_{60}H_{68}O_4N_{12}Cl_{10}Zn$, triclinic, $P\bar{1}$ (no. 2), a = 8.816 (2) Å, b = 13.688 (4) Å, c = 15.169 (4) Å, α = 91.085 (5)°, β = 98.609 (4)°, γ = 106.874 (5)°, V = 1728.2 (8) Å^3, Z = 1, $R_{gt}(F)$ = 0.0615, $wR_{ref}(F^2)$ = 0.1709, T = 296 (2) K.

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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.

Table 1: Data collection and handling.

Crystal:	Colourless needle
Size	0.35 × 0.28 × 0.20 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.80 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max}, completeness:	27.5°, 99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	9820, 7193, 0.035
Criterion for I_{obs}, $N(hkl)_{gt}$:	I_{obs} > 2 σ(I_{obs}), 4307
$N(param)_{refined}$:	396
Programs:	Bruker [1], SHELX [2–4], Diamond [5]

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

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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	0.3095 (5)	0.1584 (3)	−0.0399 (3)	0.0385 (9)
H1	0.373805	0.124130	−0.007348	0.046*
C2	0.1174 (5)	0.2066 (3)	−0.0967 (3)	0.0545 (12)
H2	0.012935	0.210183	−0.110855	0.065*
C3	0.5203 (5)	0.2766 (3)	−0.1148 (3)	0.0355 (9)
C4	0.6603 (5)	0.2802 (3)	−0.0436 (3)	0.0382 (9)
H4	0.755427	0.294546	−0.072950	0.046*
C5	0.6968 (5)	0.3632 (3)	0.0323 (3)	0.0480 (11)
C6	0.8594 (6)	0.3671 (5)	0.0868 (3)	0.0790 (17)
H6A	0.853424	0.301705	0.110415	0.118*
H6B	0.940459	0.383417	0.049163	0.118*
H6C	0.886359	0.418524	0.135207	0.118*
C7	0.5709 (6)	0.3416 (4)	0.0951 (3)	0.0643 (14)
H7A	0.601260	0.395185	0.141844	0.096*
H7B	0.467976	0.338972	0.061865	0.096*
H7C	0.564858	0.277318	0.120726	0.096*
C8	0.7082 (8)	0.4663 (4)	−0.0084 (4)	0.0804 (18)
H8A	0.606201	0.463880	−0.042668	0.121*
H8B	0.737068	0.519541	0.038538	0.121*
H8C	0.788471	0.480063	−0.046634	0.121*
C9	0.5296 (5)	0.3114 (3)	−0.1958 (3)	0.0394 (9)
H9	0.435022	0.311765	−0.232150	0.047*
C10	0.6809 (5)	0.3491 (3)	−0.2307 (2)	0.0377 (9)
C11	0.7349 (5)	0.4485 (3)	−0.2572 (3)	0.0404 (10)
C12	0.8831 (5)	0.4860 (3)	−0.2856 (3)	0.0463 (11)
H12	0.917546	0.553146	−0.301742	0.056*
C13	0.9762 (5)	0.4232 (3)	−0.2894 (3)	0.0440 (10)
C14	0.9242 (5)	0.3218 (4)	−0.2693 (3)	0.0490 (11)
H14	0.986614	0.278295	−0.274730	0.059*
C15	0.7786 (5)	0.2874 (3)	−0.2413 (3)	0.0470 (11)
H15	0.742807	0.219060	−0.228620	0.056*
C16	−0.1778 (5)	0.0716 (3)	0.1402 (3)	0.0408 (10)
H16	−0.276896	0.027587	0.114134	0.049*
C17	0.0628 (5)	0.1546 (4)	0.1669 (3)	0.0532 (12)
H17	0.170283	0.179519	0.160419	0.064*
C18	−0.2635 (5)	0.1365 (3)	0.2736 (2)	0.0357 (9)
C19	−0.3688 (5)	0.0373 (3)	0.3015 (3)	0.0411 (10)
H19	−0.453724	0.053206	0.328616	0.049*
C20	−0.2806 (6)	−0.0175 (3)	0.3701 (3)	0.0550 (12)
C21	−0.4128 (8)	−0.1043 (4)	0.4023 (4)	0.0880 (19)
H21A	−0.485407	−0.075649	0.427395	0.132*
H21B	−0.364086	−0.139631	0.446952	0.132*
H21C	−0.470834	−0.151538	0.352649	0.132*
C22	−0.1670 (7)	−0.0629 (4)	0.3309 (4)	0.0804 (17)
H22A	−0.118775	−0.098463	0.375444	0.121*
H22B	−0.084582	−0.009207	0.311037	0.121*
H22C	−0.225095	−0.109905	0.281056	0.121*
C23	−0.1926 (8)	0.0581 (4)	0.4499 (3)	0.0831 (19)
H23A	−0.110398	0.112572	0.430892	0.125*
H23B	−0.144591	0.023316	0.495299	0.125*
H23C	−0.267600	0.085783	0.473599	0.125*
C24	−0.2577 (5)	0.2303 (3)	0.3020 (2)	0.0417 (10)
H24	−0.180027	0.284269	0.283518	0.050*
C25	−0.3616 (5)	0.2572 (3)	0.3597 (3)	0.0410 (10)
C26	−0.2962 (5)	0.3157 (3)	0.4403 (3)	0.0480 (11)
C27	−0.3903 (7)	0.3485 (3)	0.4918 (3)	0.0584 (13)
H27	−0.344315	0.387879	0.544966	0.070*
C28	−0.5523 (6)	0.3221 (4)	0.4635 (3)	0.0564 (12)
C29	−0.6224 (6)	0.2630 (3)	0.3853 (3)	0.0539 (12)
H29	−0.733012	0.243995	0.367139	0.065*
C30	−0.5256 (5)	0.2330 (3)	0.3353 (3)	0.0487 (11)
H30	−0.572831	0.194226	0.281937	0.058*
Cl1	−0.24077 (13)	0.02300 (8)	−0.10474 (7)	0.0482 (3)
Cl2	0.61992 (16)	0.53033 (10)	−0.25017 (10)	0.0696 (4)
Cl3	1.16608 (14)	0.47010 (11)	−0.31778 (8)	0.0666 (4)
Cl4	−0.09040 (16)	0.34804 (10)	0.47578 (8)	0.0685 (4)
Cl5	−0.6682 (2)	0.36489 (13)	0.52899 (11)	0.0929 (5)
N1	0.1551 (4)	0.1376 (2)	−0.0416 (2)	0.0381 (8)
N2	0.3638 (4)	0.2358 (2)	−0.0911 (2)	0.0366 (8)
N3	0.2363 (4)	0.2675 (3)	−0.1285 (3)	0.0550 (10)
N4	−0.0454 (4)	0.0858 (3)	0.1074 (2)	0.0406 (8)
N5	−0.1522 (4)	0.1287 (2)	0.2163 (2)	0.0383 (8)
N6	0.0069 (4)	0.1841 (3)	0.2345 (2)	0.0569 (10)
O1	0.6440 (4)	0.1836 (2)	−0.00531 (19)	0.0490 (7)
H1A	0.674505	0.146608	−0.037272	0.074*
O2	−0.4437 (3)	−0.0320 (2)	0.22619 (19)	0.0493 (8)
H2A	−0.526311	−0.019933	0.203496	0.074*
Zn	0.000000	0.000000	0.000000	0.03525 (19)

dissolved in methanol (10 mL). Then, Zinc chloride (0.136 g, 0.100 mmol) was added. Reaction was allowed to stir at room temperature for 2 h. Colorless needle crystals of the title compound were obtained by slow evaporation from propanone.

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

The complexes containing transition metal and various 1,2,4-triazole ligands have been extensively investigated because of their novel structures and potential applications in different fields, especially in pharmaceutical industry and agriculture [6, 7]. The pharmacological and toxicological properties of many drugs are improved when they form Zn(II) complexes [7–9]. As a broad spectrum

systemic 1,2,4-triazole fungicide, diniconazole (*E*)-(*RS*)-1-(2,4-dichlorophenyl)-4,4-dimethyl-2-(1*H*-1,2,4-triazol-1-yl) pent-1-en-3-ol, has been widely used to control various fungi in many kinds of crops by inhibiting steroid demethylation [10, 11].

The asymmetric unit of the title structure contains a half Zn(II) cation, one chloride and two diniconazole molecules to construct a new mononuclear complex. The title compex is isomorphous to other transition metal compexes using the same triazole ligand [12, 13]. The Zn(II) cation is six-coordinated by two chlorido ligands and four triazole ligands. The Zn–N length (Zn–N1 = 2.151 (3) Å, Zn–N4 = 2.143 (3) Å), Zn–Cl length (Zn–Cl1 = 2.5546 (11) Å), the N1–Zn–N4, N1–Zn–N4^{i}, N1–Zn–Cl1, N4–Zn–Cl1, N1–Zn–Cl1^{i}, and N4–Zn–Cl1^{i} bond angles of 90.32 (12)°, 89.68 (12)°, 90.88 (9)°, 91.69 (9)°, 89.12 (9)°, and 88.31 (9)°, respectively (symmetry code: (i) $-x$, $-y$, $-z+1$) are all in the expected ranges. The Zn(II) cation is the center of symmetry so the bond angle of N1–Zn–N1^{ii}, N4–Zn–N4^{ii}, and Cl1–Zn–Cl1^{ii} is 180°. These parameters are in agreement with closely related Zn(II) complexes [14–16]. The title compound forms a O1–H1A···Cl1^{ii} ($d_{O1\cdots Cl1}$ = 3.125 (3) Å, 169.2°, symmetry code: (ii) $x+1$, y, z) and O2–H2A···Cl1^{iii} ($d_{O2\cdots Cl1}$ = 3.133 (3) Å, 162.1°, symmetry code: (iii) $-x-1$, $-y$, $-z$) hydrogen bond forming a chain along the a-axis.

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

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