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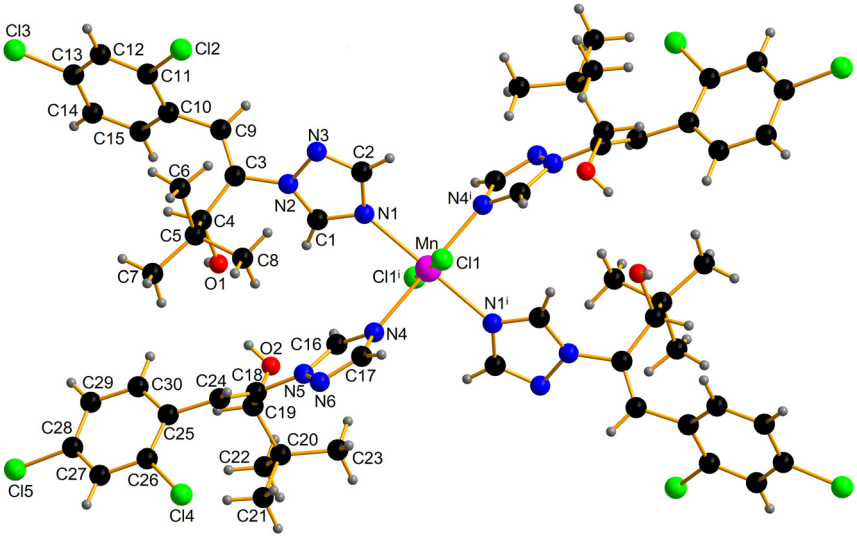
# Crystal structure of dichlorido-tetrakis(1-(2,4-dichlorophenyl)-4,4-dimethyl-2-(1,2,4-triazol-1-yl)pent-1-en-3-ol-$\kappa^1N$) manganese(II), $C_{60}H_{68}O_4N_{12}Cl_{10}Mn$

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**Abstract**

$C_{60}H_{68}O_4N_{12}Cl_{10}Mn$, triclinic, $P\bar{1}$ (no. 2), $a$ = 8.9262(11) Å, $b$ = 13.7013(18) Å, $c$ = 15.330(2) Å, $\alpha$ = 91.414(2)°, $\beta$ = 98.951(2)°, $\gamma$ = 106.688(2)°, $V$ = 1769.3(4) Å$^3$, $Z$ = 1, $R_{gt}(F)$ = 0.0443, $wR_{ref}(F^2)$ = 0.1222, $T$ = 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.

## 1 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, 0.2 mmol) was dissolved in methanol (10 mL). Then, manganese chloride tetrahydrate (0.198 g, 0.1 mmol) was added. Reaction was allowed to stir at room temperature for 2 h. Pink needle crystal of the title compound was obtained by slow evaporation from propanone.

**Table 1:** Data collection and handling.

| | |
|---|---|
| Crystal: | Pink needle |
| Size: | 0.35 × 0.27 × 0.16 mm |
| Wavelength: | Mo *K*α radiation (0.71073 Å) |
| $\mu$: | 0.62 mm$^{-1}$ |
| Diffractometer, scan mode: | Bruker APEX-II, $\varphi$ and $\omega$ |
| $\theta_{max}$, completeness: | 28.4°, 99 % |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$, $R_{int}$: | 10,534, 7756, 0.023 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\sigma(I_{obs})$, 5739 |
| $N(param)_{refined}$: | 402 |
| Programs: | Bruker [1], SHELX [2–4], Diamond [5] |

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

| Atom | x | y | z | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Mn | 0.500000 | 0.500000 | 0.000000 | 0.03029 (12) |
| Cl1 | 0.74024 (7) | 0.47851 (5) | 0.10640 (4) | 0.04816 (17) |
| Cl2 | 0.39941 (9) | 0.85111 (6) | 0.47832 (5) | 0.0691 (2) |
| Cl3 | −0.17640 (12) | 0.86298 (8) | 0.53008 (7) | 0.0950 (3) |
| Cl4 | −0.12160 (9) | −0.03241 (6) | 0.24942 (6) | 0.0697 (2) |
| Cl5 | −0.66239 (8) | 0.02985 (6) | 0.31674 (5) | 0.0654 (2) |
| N1 | 0.4520 (2) | 0.59086 (16) | 0.11160 (12) | 0.0421 (5) |
| N2 | 0.3430 (2) | 0.63165 (15) | 0.21983 (12) | 0.0370 (4) |
| N3 | 0.4992 (2) | 0.68953 (19) | 0.23896 (14) | 0.0567 (6) |
| N4 | 0.3399 (2) | 0.35657 (15) | 0.04347 (13) | 0.0404 (5) |
| N5 | 0.1333 (2) | 0.26191 (14) | 0.09368 (12) | 0.0353 (4) |
| N6 | 0.2576 (2) | 0.22805 (18) | 0.13018 (16) | 0.0565 (6) |
| O1 | 0.0546 (2) | 0.46907 (13) | 0.22728 (11) | 0.0488 (4) |
| H1A | −0.025303 | 0.482234 | 0.203204 | 0.073* |
| O2 | −0.1437 (2) | 0.31610 (13) | 0.00783 (11) | 0.0483 (4) |
| H2A | −0.171496 | 0.354001 | 0.039883 | 0.072* |
| C1 | 0.3191 (3) | 0.57584 (18) | 0.14375 (14) | 0.0386 (5) |
| H1 | 0.221443 | 0.532060 | 0.116847 | 0.046* |
| C2 | 0.5575 (3) | 0.6611 (2) | 0.17188 (17) | 0.0549 (7) |
| H2 | 0.663701 | 0.687415 | 0.166468 | 0.066* |
| C3 | 0.2310 (3) | 0.63892 (18) | 0.27668 (13) | 0.0356 (5) |
| C4 | 0.1290 (3) | 0.53985 (17) | 0.30288 (15) | 0.0388 (5) |
| H4 | 0.044774 | 0.555014 | 0.329732 | 0.047* |
| C5 | 0.2179 (3) | 0.4843 (2) | 0.37108 (17) | 0.0535 (7) |
| C6 | 0.3072 (5) | 0.5602 (3) | 0.4504 (2) | 0.0875 (12) |
| H6A | 0.346002 | 0.524212 | 0.497474 | 0.131* |
| H6B | 0.236568 | 0.593642 | 0.470492 | 0.131* |
| H6C | 0.394910 | 0.610243 | 0.432868 | 0.131* |
| C7 | 0.0910 (5) | 0.3976 (3) | 0.4027 (2) | 0.0889 (11) |
| H7A | 0.032477 | 0.350621 | 0.353247 | 0.133* |
| H7B | 0.019826 | 0.425568 | 0.428805 | 0.133* |
| H7C | 0.141239 | 0.362286 | 0.445936 | 0.133* |
| C8 | 0.3316 (4) | 0.4390 (3) | 0.3313 (2) | 0.0777 (10) |
| H8A | 0.422304 | 0.493051 | 0.321934 | 0.117* |
| H8B | 0.278673 | 0.401944 | 0.275779 | 0.117* |
| H8C | 0.365415 | 0.393569 | 0.371155 | 0.117* |
| C9 | 0.2349 (3) | 0.73235 (18) | 0.30434 (14) | 0.0399 (5) |
| H9 | 0.310404 | 0.786452 | 0.286010 | 0.048* |
| C10 | 0.1304 (3) | 0.75907 (17) | 0.36181 (14) | 0.0377 (5) |
| C11 | 0.1950 (3) | 0.81740 (18) | 0.44173 (15) | 0.0443 (6) |
| C12 | 0.1021 (4) | 0.8499 (2) | 0.49383 (17) | 0.0536 (7) |
| H12 | 0.147705 | 0.889827 | 0.546484 | 0.064* |
| C13 | −0.0594 (4) | 0.8214 (2) | 0.46547 (18) | 0.0549 (7) |
| C14 | −0.1295 (3) | 0.7634 (2) | 0.38707 (18) | 0.0522 (6) |
| H14 | −0.238824 | 0.745256 | 0.368641 | 0.063* |
| C15 | −0.0328 (3) | 0.7329 (2) | 0.33642 (16) | 0.0465 (6) |
| H15 | −0.079151 | 0.693518 | 0.283565 | 0.056* |
| C16 | 0.1857 (3) | 0.33809 (17) | 0.04256 (15) | 0.0382 (5) |
| H16 | 0.122600 | 0.373076 | 0.010868 | 0.046* |
| C17 | 0.3766 (3) | 0.2874 (2) | 0.09781 (19) | 0.0582 (7) |
| H17 | 0.479182 | 0.282224 | 0.111296 | 0.070* |
| C18 | −0.0221 (2) | 0.22234 (16) | 0.11665 (14) | 0.0334 (5) |
| C19 | −0.1621 (3) | 0.21944 (17) | 0.04521 (14) | 0.0366 (5) |
| H19 | −0.256270 | 0.205691 | 0.073748 | 0.044* |
| C20 | −0.1979 (3) | 0.13581 (19) | −0.03121 (16) | 0.0457 (6) |
| C21 | −0.2114 (4) | 0.0322 (2) | 0.0083 (2) | 0.0796 (10) |
| H21A | −0.289310 | 0.019673 | 0.046555 | 0.119* |
| H21B | −0.110470 | 0.033142 | 0.041584 | 0.119* |
| H21C | −0.242696 | −0.021016 | −0.038674 | 0.119* |
| C22 | −0.3596 (4) | 0.1328 (3) | −0.0856 (2) | 0.0756 (9) |
| H22A | −0.388540 | 0.080191 | −0.132923 | 0.113* |
| H22B | −0.352414 | 0.197658 | −0.109871 | 0.113* |
| H22C | −0.438706 | 0.118846 | −0.048048 | 0.113* |
| C23 | −0.0740 (4) | 0.1573 (3) | −0.09279 (18) | 0.0668 (8) |
| H23A | 0.025435 | 0.153346 | −0.061103 | 0.100* |
| H23B | −0.060715 | 0.224489 | −0.113218 | 0.100* |
| H23C | −0.109114 | 0.107681 | −0.142594 | 0.100* |
| C24 | −0.0321 (3) | 0.18729 (18) | 0.19659 (15) | 0.0401 (5) |
| H24 | 0.061218 | 0.186407 | 0.232829 | 0.048* |
| C25 | −0.1832 (3) | 0.14961 (18) | 0.23122 (14) | 0.0379 (5) |
| C26 | −0.2368 (3) | 0.04964 (19) | 0.25606 (15) | 0.0411 (5) |
| C27 | −0.3814 (3) | 0.01249 (19) | 0.28457 (15) | 0.0458 (6) |
| H27 | −0.414770 | −0.054332 | 0.300645 | 0.055* |
| C28 | −0.4751 (3) | 0.0768 (2) | 0.28862 (15) | 0.0442 (6) |
| C29 | −0.4223 (3) | 0.1778 (2) | 0.26984 (16) | 0.0496 (6) |
| H29 | −0.483036 | 0.221722 | 0.276065 | 0.060* |
| C30 | −0.2775 (3) | 0.21255 (19) | 0.24159 (16) | 0.0465 (6) |
| H30 | −0.241926 | 0.280615 | 0.229091 | 0.056* |

# 2 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).

# 3 Comment

Triazole fungicides have the advantages of high efficiency, broad spectrum, low toxicity to nontarget organisms, and low resistance. Triazole fungicides can be used to control fungal diseases, such as powdery mildews, rusts, and many leaf spot fungi on a variety of plants [6]. In recent years, they have been widely used in the food and environmental fields [7, 8]. Diniconazole (*E*)-(*RS*)-1-(2,4-dichlorophenyl)-4,4-dimethyl-2-(1*H*-1,2,4-triazol-1-yl) pent-1-en-3-ol is a chiral triazole fungicide with protective, therapeutic, and eradicative effects. Its mode of action is to inhibit the demethylation of steroids, which play an important role in the ergosterol biosynthesis of basidiomycetes and ascomycetes, it has strong bactericidal activity to ascomycotina,

basidiomycotina, and deuteromycotina [9]. After application, diniconazole can be absorbed by various parts of the plant, and it has been widely used in cereals, fruit trees, vegetables, and so on [10]. The pharmacological and toxicological properties of many drugs are improved when they form metal complexes [11–14]. In this paper, a new diniconazole Mn(II) complex is described.

The asymmetric unit of the title structure contains a half Mn(II) cation, one chlorine anion and two diniconazole molecules to construct a new mononuclear complex. The Mn(II) cation is six-coordinated by two chlorido ligands and four triazole ligands. The Mn–N length (Mn–N1 = 2.2559(18) Å, Mn–N4 = 2.2576(18) Å) and Mn–Cl length (Mn–Cl1 = 2.5775(6) Å), the N1–Mn–N4, N1–Mn–N4$^{i}$, N1–Mn–Cl1, N4–Mn–Cl1, N1–Mn–Cl1$^{i}$, and N4–Mn–Cl1$^{i}$ bond angles of 89.30(7)°, 90.70(7)°, 87.99(5)°, 90.84(5)°, 92.01(5)°, and 89.16(5)°, respectively (symmetry code: (i) $-x + 1, -y + 1, -z$). Mn(II) cation is the center of symmetry of the title compound, so the bond angle of N1–Mn–N1$^{i}$, N4–Mn–N4$^{i}$, and Cl1–Mn–Cl1$^{i}$ is 180°. These are in agreement with closely related Mn(II) complexes reported [15–18]. The title compound through O1–H1A$\cdots$Cl1$^{ii}$ ($d_{O1\cdots Cl1}$ = 3.1505(17) Å, 163.2°, symmetry code: (ii) $x-1, y, z$) and O2–H2A$\cdots$Cl1$^{ii}$ ($d_{O2\cdots Cl1}$ = 3.1552(18) Å, 168.8°) hydrogen bond forming a one-dimensional (1D) chain along the *a*-axis.

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

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

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