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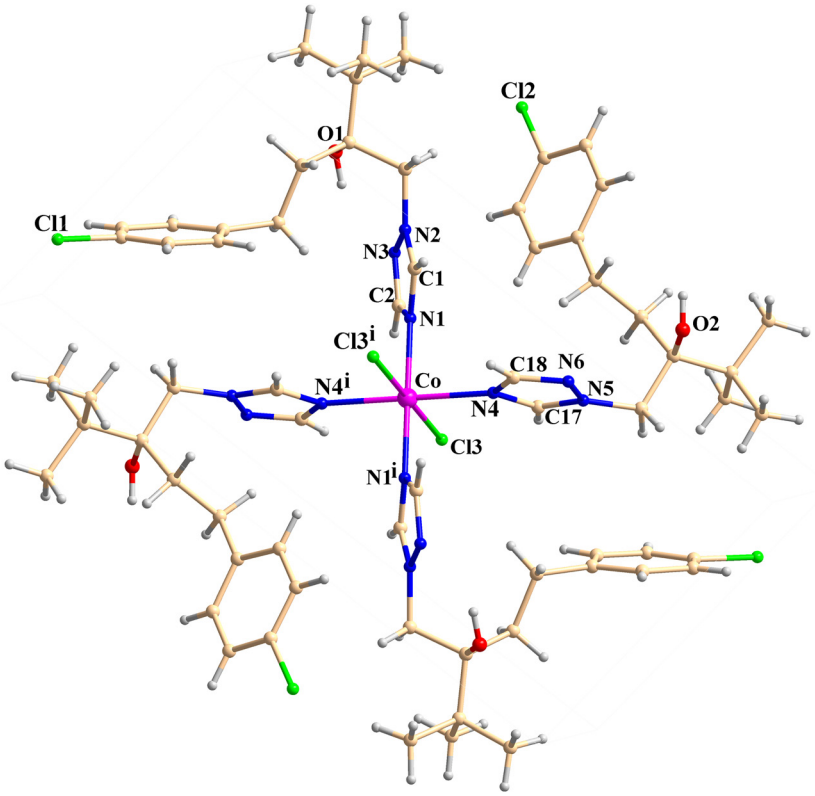
Crystal structure of dichlorido–tetrakis{3-((1*H*-1,2,4-triazol-1-yl)methyl)-1-(4-chlorophenyl)-4,4-dimethylpentan-3-ol-κ^{1}N}cobalt(II), $C_{64}H_{88}O_4N_{12}Cl_6Co$



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Abstract

$C_{64}H_{88}O_4N_{12}Cl_6Co$, triclinic, $P\bar{1}$, a = 9.1414(10) Å, b = 12.0301(14) Å, c = 17.521(2) Å, α = 80.372(2)°, β = 78.559(2)°, γ = 69.025(2)°, V = 1753.6(3) Å^3, Z = 1, $R_{gt}(F)$ = 0.0665, $wR_{ref}(F^2)$ = 0.1793, T = 296(2) K.

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The molecular structure is shown in the figure. Table 1 contains the crystallographic data and the list of the atoms including atomic coordinates and displacement parameters can be found in the cif-file attached to this article.

1 Source of material

The (*RS*)-1-(4-chlorophenyl)-4,4-dimethyl-3-(1*H*-1-ylmethyl) pentan-3-ol (0.3078 g, 1.00 mmol) was dissolved in ethanol (10 mL). Subsequently, cobalt chloride hexahydrate (0.5949 g, 0.25 mmol) was added to the solution. The reaction mixture was stirred at room temperature for 2 h. The red block

Table 1: Data collection and handling.

Crystal:	Red block
Size:	0.32 × 0.30 × 0.25 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.53 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω scans
θ_{max}, completeness:	25.0°, 99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	8852, 6111, 0.039
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 3665
$N(param)_{refined}$:	402
Programs:	Bruker,[1] SHELX,[2–4] Diamond[5]

crystals of the target compound were obtained through slow evaporation of the ethanol.

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) = 1.5U_{eq} (C), C–H = 0.98 Å (methine), U_{iso} (H) = 1.2U_{eq} (C), C–H = 0.93 Å (aromatic and alkenyl), U_{iso} (H) = 1.2U_{eq} (C), and O–H = 0.82 Å (hydroxyl), U_{iso} (H) = 1.5U_{eq} (O).

3 Comment

Tebuconazole, (RS)-3-((1H-1,2,4-triazol-1-yl)methyl)-1-(4-chlorophenyl)-4,4-dimethylpentan-3-ol, a systemic 1,2,4-triazole fungicide, has been extensively utilized for controlling mildews and rusts on cereal grains, fruits, vegetables, and ornamental plants.[6,7] However, the widespread application of tebuconazole has resulted in significant environmental contamination and the rapid emergence of resistant strains.[8–10] Recent studies have shown that the complexation of 1,2,4-triazoles with transition metals represents an attractive approach to enhance the biological activities.[11–15] Consequently, this paper introduces a novel tebuconazole Co(II) complex designed to improve antifungal efficacy and mitigate the environmental issues associated with tebuconazole.

The asymmetric unit of the title complex contains one half of Co(II) cation, one chloride anion and two tebuconazole molecules. The Co(II) cation is six-coordinated by two chloride atoms and four triazole ligands. The Co–N lengths (Co–N1 = 2.122(4) Å, Co–N4 = 2.191(4) Å), Co–Cl length (Co–Cl3 = 2.4791(13) Å), and the bond angles of N1–Co–N4, N1–Co–$N4^i$, N1–Co–Cl, N1–Co–Cl^i, N4–Co–Cl, and N4–Co–Cl^i (93.12(15)°, 86.88(15)°, 90.16(12)°, 89.84(11)°, 90.79(11)°, and 89.21(10)°, respectively, symmetry code: (i) $-x+1, -y+1, -z+1$) are all in the expected range. Co(II) cation is the center of the symmetry of the title compound, so all the bond angles of N1–Co–$N1^i$, N4–Co–$N4^i$, and Cl–Co–Cl^i are 180°. These are in agreement with the reported closely related Co(II) complexes.[16,17] There are two kinds of intramolecular hydrogen bonds of O1–H1···N2 ($d_{O1\cdots N2}$ = 2.949(5) Å, 111.9°) and O1–H1···N3 ($d_{O1\cdots N3}$ = 2.837(6) Å, 143.5°) in the crystal structure, which are generated by O1 atom from one hydroxyl group as hydrogen bond donor to N2 and N3 of the triazole ring. Moreover, O2 atom from the other unsymmetrical hydroxyl group acts as hydrogen bond donor to Cl3 atom from the adjacent molecule, generating a strong intermolecular hydrogen bond of O1–H1···$Cl3^{ii}$ ($d_{O1\cdots Cl}$ = 3.284(3) Å, 155.5°, symmetry code: (ii) x –1, y, z). The intermolecular hydrogen bond forms a one-dimensional (1D) chain along the c-axis.

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