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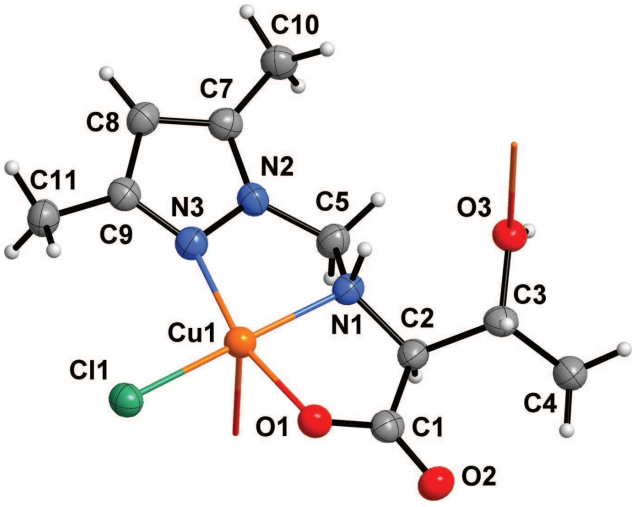
Crystal structure of the coordination polymer *catena*-poly[chlorido-{μ_2-2-(((3,5-dimethyl-1*H*-pyrazol-1-yl)methyl)amino)-3-hydroxybutanoato-κ^4*N*,*N*,*O*:*O*'}copper(II)], $C_{11}H_{16}ClCuN_2O_3$



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Abstract

$C_{11}H_{16}ClCuN_2O_3$, monoclinic, $P2_1/n$ (no. 14), $a = 5.6017(4)$ Å, $b = 10.7601(8)$ Å, $c = 10.4036(8)$ Å, $\beta = 95.697(2)°$, $V = 623.98(8)$ Å^3, $Z = 2$, $R_{gt}(F) = 0.0321$, $wR_{ref}(F^2) = 0.0833$, $T = 100(1)$ K.

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The crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

Preparation of the copper(II) complex: 2-(((3,5-dimethyl-2*H*-pyrrol-2-yl)methyl)amino)-3-hydroxybutanoic acid (0.335 g, 1 mmol) in 20 mL of EtOH was added to $CuCl_2{\cdot}2H_2O$ (0.17 g, 1 mmol) dissolved in 10 mL of EtOH. The reaction mixture was left at room temperature for couple of days until the complete evaporation of solvent. The blue powder was washed several times with THF. Suitable crystals were obtained by recrystallization from a mixture of Ether/EtOH. A blue crystal was obtained with a period of 6 days. Yield (22%).

Table 1: Data collection and handling.

Crystal:	Blue block
Size:	0.07 × 0.05 × 0.02 mm
Wavelength:	Cu $K\alpha$ radiation (1.54178 Å)
μ:	4.5 mm^{-1}
Diffractometer, scan mode:	Bruker X8 PROSPECTOR APEX2, φ and ω-scans
θ_{max}, completeness:	66.9°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	14015, 2145, 0.027
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2141
$N(param)_{refined}$:	169
Programs:	Bruker programs [1], SHELX [2]

Experimental details

Hydrogen atoms were placed at the calculated positions and refined using a riding model with $U_{iso}(H) = 1.2U_{eq}$ or $1.5U_{eq}$ of the adjacent non-hydrogen atom. H3 atom position was localized from the difference map and refined with the DFIX option N—H = 0.87 Å and $U_{iso}(H) = 1.5U_{eq}$(O3).

Discussion

Amino acids can bind transition metal like other chelate ligands in monodentate, bidentate and tridentate modes [3, 4]. The coordination of metals with amino acids especially with copper has been the subject of many studies because they are simple systems that can serve as a model for metallo-proteins [5]. Amino acids-metal complexes have been used as antibacterial and anticancer drugs [2–7]. The research area of coordination polymers was established by Robson and Hoskins about 30 years ago [8]. Design and synthesis of coordination polymers have attracted interests for their unprecedented and possibly useful physical properties [6–10].

Each Cu(II) atom in the synthesized coordination polymers is coordinated by five donor atoms: one Cl, two

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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}
Cu1	0.10252(8)	0.39832(5)	0.65832(5)	0.0288(2)
Cl1	−0.20257(16)	0.27451(9)	0.69674(9)	0.0323(2)
O1	0.1517(5)	0.3154(3)	0.4961(3)	0.0322(6)
O2	0.2738(6)	0.3585(3)	0.3046(3)	0.0375(7)
O3	0.8352(5)	0.5510(3)	0.5388(3)	0.0313(6)
H3	0.847(10)	0.6267(19)	0.523(6)	0.047*
N1	0.4025(6)	0.4881(3)	0.6216(3)	0.0294(7)
H1	0.5431	0.4386	0.6599	0.035*
N3	0.1435(6)	0.4966(3)	0.8214(3)	0.0303(7)
C1	0.2687(7)	0.3812(4)	0.4195(4)	0.0308(8)
C2	0.4129(7)	0.4932(4)	0.4798(3)	0.0295(8)
H2	0.3344	0.5718	0.4460	0.035*
C3	0.6749(7)	0.4901(4)	0.4421(4)	0.0301(8)
H3A	0.7250	0.4011	0.4385	0.036*
C4	0.6950(7)	0.5469(4)	0.3101(4)	0.0357(9)
H4A	0.6374	0.6329	0.3093	0.054*
H4B	0.5976	0.4987	0.2443	0.054*
H4C	0.8630	0.5456	0.2914	0.054*
C5	0.4052(7)	0.6076(4)	0.6885(4)	0.0337(9)
H5A	0.2959	0.6673	0.6400	0.040*
H5B	0.5691	0.6431	0.6979	0.040*
N2	0.3241(6)	0.5817(4)	0.8155(3)	0.0315(7)
C7	0.3881(7)	0.6325(4)	0.9323(4)	0.0305(8)
C8	0.2436(7)	0.5786(4)	1.0170(4)	0.0312(8)
H8	0.2454	0.5953	1.1067	0.037*
C9	0.0940(7)	0.4946(4)	0.9446(4)	0.0299(8)
C10	0.5825(7)	0.7263(4)	0.9557(4)	0.0353(9)
H10A	0.7330	0.6915	0.9310	0.053*
H10B	0.6020	0.7484	1.0475	0.053*
H10C	0.5406	0.8007	0.9040	0.053*
C11	−0.0910(7)	0.4130(5)	0.9927(4)	0.0351(9)
H11A	−0.2486	0.4526	0.9766	0.053*
H11B	−0.0537	0.3995	1.0857	0.053*
H11C	−0.0929	0.3330	0.9476	0.053*

O and two N atoms. The apical position of copper center was occupied by O3 atom from the hydroxyl group. A Jahn-Teller effect of the Cu(II) ion was detected on Cu–O3 bond length (2.473 Å). The Cu(II) centers lie in the center of the square (N, O, Cl, N), the O3 atom is positioned perpendicular to such a square plane giving a slightly distorted-square pyramid (*cf.* the figure).

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