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Crystal structure of diacetato- $\kappa^1\text{O}$ -diethanol- $\kappa^1\text{O}$ -bis(μ_2 -2-(((2-hydroxyethyl)imino)methyl)-5-methoxyphenolato- $\kappa^4\text{O},\text{N},\text{O}':\text{O}''$)dinickel(II), $\text{C}_{28}\text{H}_{42}\text{Ni}_2\text{N}_2\text{O}_{12}$

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:	Green block
Size:	$0.05 \times 0.04 \times 0.02$ mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	1.24 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max} , completeness:	25.0° , >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	14072, 2825, 0.032
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2656
$N(\text{param})_{\text{refined}}$:	202
Programs:	Bruker [1], SHELX [2, 3]

Source of material

The ligand was synthesized according to the reference method [4]. All other reagents were commercially available and used as purchased. A mixture of 2-(((2-hydroxyethyl)imino)methyl)-5-methoxyphenol (78.08 mg, 0.2 mmol) nickel(II) acetate (0.2 mmol) and ethanol (10 mL) was heated at 60°C for 10 h, and then cooled to room temperature. The resulting black block crystals of the title compound were obtained and washed with distilled water. The yield is ca. 35%. IR(KBr): 3257(s), 1588(s), 1559(s), 1456(s), 1455(s), 1349(s), 1286(s), 1156(s), 1115(s), 1052(s), 1001(s), 925(s), 859(s), 814(m), 761(m), 721(m), 600(m), 444(m) cm^{-1} .

Experimental details

The H atoms were geometrically placed ($\text{C}-\text{H} = 0.95\text{--}0.98$ Å) and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2\text{--}1.5 U_{\text{eq}}(\text{C})$. The ethanol ligand shows a small disorder, which was not included in the refinement.

Comment

Salicylaldehyde Schiff bases are organic ligands containing methylene amine group or imide group. Salicylaldehyde Schiff bases are important ligands in coordination chemistry. Many complexes with the Schiff bases have been synthesized [4–8]. The manganese complex with the ligand, 2-(((2-hydroxyethyl)imino)methyl)-5-methoxyphenolato,

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Abstract

$\text{C}_{28}\text{H}_{42}\text{Ni}_2\text{N}_2\text{O}_{12}$, monoclinic, $P2_1/c$ (no. 14), $a = 11.030(2)$ Å, $b = 15.138(3)$ Å, $c = 9.800(2)$ Å, $\beta = 101.439(2)^\circ$, $Z = 2$, $V = 1603.7(6)$ Å³, $R_{\text{gt}}(F) = 0.0313$, $wR_{\text{ref}}(F^2) = 0.0938$, $T = 298$ K.

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	U _{iso} [*] /U _{eq}
C1	1.0467(3)	0.3651(2)	0.9782(3)	0.0604(8)
H1A	1.0254	0.3117	1.0206	0.091*
H1B	1.0938	0.4026	1.0482	0.091*
H1C	1.0951	0.3511	0.9097	0.091*
C2	0.8638(2)	0.37222(16)	0.7989(2)	0.0368(5)
C3	0.8869(2)	0.29115(17)	0.7414(3)	0.0402(5)
H3	0.9565	0.2579	0.7790	0.048*
C4	0.8031(2)	0.26223(16)	0.6273(3)	0.0388(5)
H4	0.8178	0.2083	0.5883	0.047*
C5	0.69636(19)	0.30943(14)	0.5659(2)	0.0301(5)
C6	0.67430(19)	0.39308(13)	0.6253(2)	0.0257(4)
C7	0.7595(2)	0.42137(14)	0.7418(3)	0.0334(5)
H7	0.7461	0.4750	0.7828	0.040*
C8	0.6153(2)	0.26823(14)	0.4497(2)	0.0331(5)
H8	0.6393	0.2132	0.4223	0.040*
C9	0.4404(2)	0.24772(16)	0.2670(3)	0.0413(6)
H9A	0.3736	0.2178	0.2993	0.050*
H9B	0.4918	0.2036	0.2345	0.050*
C10	0.3887(3)	0.31105(17)	0.1502(3)	0.0442(6)
H10A	0.4542	0.3299	0.1038	0.053*
H10B	0.3258	0.2814	0.0823	0.053*
C11	0.6832(4)	0.4405(2)	0.2348(4)	0.0696(10)
H11A	0.6611	0.3800	0.2078	0.084*
H11B	0.7578	0.4389	0.3064	0.084*
C12	0.7088(6)	0.4894(3)	0.1122(5)	0.122(2)
H12A	0.6487	0.4733	0.0311	0.183*
H12B	0.7901	0.4747	0.0982	0.183*
H12C	0.7041	0.5518	0.1282	0.183*
C13	0.2036(2)	0.37494(17)	0.4552(3)	0.0422(6)
C14	0.1125(3)	0.3830(3)	0.5503(4)	0.0836(13)
H14A	0.0332	0.3615	0.5036	0.125*
H14B	0.1053	0.4439	0.5751	0.125*
H14C	0.1408	0.3488	0.6330	0.125*
N1	0.51419(17)	0.29955(12)	0.38070(19)	0.0314(4)
Ni1	0.45452(2)	0.42393(2)	0.39522(2)	0.02499(13)
O1	0.93663(19)	0.40964(15)	0.9129(2)	0.0584(6)
O2	0.57629(14)	0.44279(10)	0.57540(15)	0.0272(3)
O3	0.33595(16)	0.38631(11)	0.20490(16)	0.0376(4)
H3A	0.2925	0.3539	0.2473	0.045*
O4	0.58797(17)	0.47857(12)	0.28946(18)	0.0471(4)
H4A	0.5385	0.4754	0.2112	0.057*
O5	0.31329(15)	0.40117(11)	0.50371(17)	0.0355(4)
O6	0.16775(17)	0.34237(15)	0.3380(2)	0.0587(5)

which is very similar to the title complex has been synthesized [9]. The title compound consist of two Schiff base ligands, two nickel atoms, two acetate groups and two ethanol molecules, arranged around an inversion center. The coordination of Ni ion is built up by the oxygen atoms from the Schiff base ligands, the acetate group and the ethanol molecule. The bond

lengths of Ni1—O2, Ni1—O3 and Ni1—N1 are 2.016, 2.132 and 2.009 Å, which are slightly longer than the corresponding bond lengths of the similar compound [10]. The coordination environment of each Ni atom is an octahedron, which is the same with the reference compound [9].

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