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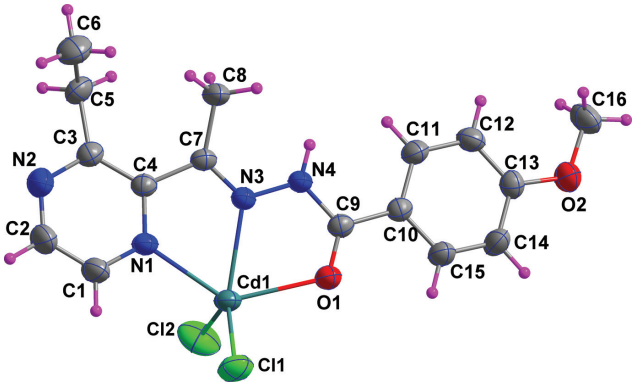
Crystal structure of dichlorido-(N′-(1-(3-ethylpyrazin-2-yl)ethylidene)-4-methoxybenzohydrazide-κ^3*N*,*N*′,*O*)cadmium(II), $C_{16}H_{18}N_4O_2Cl_2Cd$



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Abstract

$C_{16}H_{18}N_4O_2Cl_2Cd$, monoclinic, $P2_1/n$ (no. 14), $a = 9.833(2)$ Å, $b = 17.404(4)$ Å, $c = 11.694(3)$ Å, $\beta = 112.901(3)°$, $V = 1843.5(8)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0280$, $wR_{ref}(F^2) = 0.0728$, $T = 296(2)$ K.

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The crystal 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.

Source of material

4-Methoxybenzohydrazide (0.166 g, 1 mmol) and 2-acetopyrazine (0.122 g, 1 mmol) were dissolved in methanol (20 mL). The reaction mixture was refluxed for 1 h and cooled to room temperature. Then cadmium(II) chloride (0.183 g, 1 mmol) was added. After stirring for 1 h, the mixture was

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Table 1: Data collection and handling.

Crystal:	Yellow block
Size:	0.15 × 0.12 × 0.10 mm
Wavelength:	Mo *Kα* radiation (0.71073 Å)
μ:	1.49 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω-scans
θ_{max}, completeness:	25°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	15734, 3244, 0.028
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 2958
$N(param)_{refined}$:	229
Programs:	Bruker programs [1], SHELX [2]

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.47352(2)	0.55740(2)	0.23571(2)	0.03739(10)
Cl1	0.25031(9)	0.48710(5)	0.19936(9)	0.0560(2)
Cl2	0.53495(14)	0.66448(6)	0.37506(10)	0.0720(3)
O1	0.4117(2)	0.61886(13)	0.0430(2)	0.0481(5)
O2	0.4183(3)	0.82675(14)	−0.3953(2)	0.0546(6)
N1	0.6492(3)	0.46230(14)	0.3418(2)	0.0361(5)
N2	0.8846(3)	0.38111(18)	0.5031(3)	0.0570(8)
N3	0.6558(3)	0.54161(13)	0.1564(2)	0.0324(5)
N4	0.6338(3)	0.58158(14)	0.0496(2)	0.0352(5)
H4	0.6967	0.5798	0.0152	0.042*
C1	0.6408(4)	0.42534(19)	0.4377(3)	0.0476(8)
H1	0.5539	0.4275	0.4516	0.057*
C2	0.7582(4)	0.3840(2)	0.5167(3)	0.0599(10)
H2	0.7482	0.3572	0.5818	0.072*
C3	0.8971(3)	0.41819(17)	0.4059(3)	0.0392(7)
C4	0.7745(3)	0.45736(15)	0.3210(3)	0.0317(6)
C5	1.0497(3)	0.4128(2)	0.4054(3)	0.0466(8)
H5A	1.1222	0.4201	0.4892	0.056*
H5B	1.0628	0.4536	0.3541	0.056*
C6	1.0765(5)	0.3358(2)	0.3564(4)	0.0657(10)
H6A	1.0058	0.3286	0.2731	0.099*
H6B	1.0664	0.2953	0.4083	0.099*
H6C	1.1744	0.3348	0.3570	0.099*
C7	0.7666(3)	0.49699(16)	0.2046(3)	0.0314(6)
C8	0.8736(4)	0.4814(2)	0.1455(3)	0.0525(9)
H8A	0.8245	0.4864	0.0570	0.079*
H8B	0.9119	0.4303	0.1657	0.079*
H8C	0.9534	0.5177	0.1756	0.079*
C9	0.5083(3)	0.62416(15)	0.0005(3)	0.0325(6)
C10	0.4915(3)	0.67529(16)	−0.1042(3)	0.0330(6)
C11	0.6000(4)	0.68576(18)	−0.1513(3)	0.0432(7)
H11	0.6886	0.6590	−0.1161	0.052*
C12	0.5789(4)	0.73510(18)	−0.2493(3)	0.0425(7)
H12	0.6519	0.7408	−0.2806	0.051*

Table 2 (continued)

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
C13	0.4489(3)	0.77581(17)	−0.3004(3)	0.0386(7)
C14	0.3400(4)	0.7662(2)	−0.2530(3)	0.0511(8)
H14	0.2521	0.7936	−0.2871	0.061*
C15	0.3615(3)	0.71679(18)	−0.1570(3)	0.0429(7)
H15	0.2878	0.7108	−0.1265	0.052*
C16	0.5249(5)	0.8377(2)	−0.4487(4)	0.0572(9)
H16A	0.4882	0.8743	−0.5151	0.086*
H16B	0.5431	0.7896	−0.4805	0.086*
H16C	0.6152	0.8564	−0.3865	0.086*

filtered and set aside to crystallize for several days, giving yellow block crystals.

Experimental details

The structure was solved by Direct Methods and refined with the SHELX crystallographic software package [2]. The hydrogen atoms were placed at calculated positions and refined as riding atoms with isotropic displacement parameters.

Discussion

Hydrozones derived from 2-aceto-pyrazine and their metal complexes have been widely investigated mainly due to their excellent biological activities [3–5]. It is noted that the biological activities of the resulted complexes depend not only on the metal centers but also on the structures of the ligands [3, 4].

In the title crystal structure, the central cadmium(II) ion is five-coordinated to one neutral hydrazone ligand by a ON_2 donor set, and two chlorido ligands giving a distorted tetragonal-pyramidal coordination geometry with the geometric index τ value of 0.032 [6]. In the solid state, the intermolecular N—H···O hydrogen bonds link the complexes into a zig-zag chain. Bond lengths and angels are all in the expected ranges [7].

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