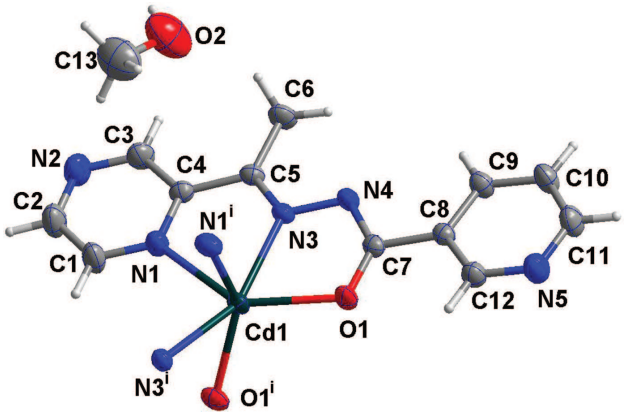
Ning Zhang, Meijie Su, Gaoyuan Xu* and Huijun Li

Crystal structure of bis(*N*-(1-(pyrazin-2-yl) ethylidene)nicotinohydrazonato-κ^3*N*,*N*′,*O*) cadmium(II) – methanol (1/1), $C_{26}H_{28}N_{10}O_4Zn$



https://doi.org/10.1515/ncrs-2017-0431
Received April 1, 2018; accepted June 7, 2018; available online June 29, 2018

Abstract

$C_{26}H_{28}N_{10}O_4Zn$, monoclinic, *C*2/*c* (no. 15), $a = 14.507(4)$ Å, $b = 16.776(5)$ Å, $c = 12.151(3)$ Å, $\beta = 108.596(4)°$, $V = 2802.8(13)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0258$, $wR_{ref}(F^2) = 0.0719$, $T = 293(2)$ K.

CCDC no.: 1847966

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

All chemicals were commercially purchased except for (*E*)-*N*′-(1-(pyrazin-2-yl)ethylidene)nicotinohydrazide (*HL*) which was synthesized according to the literature [1]. A mixture of *HL* (0.05 mmol, 12.1 mg) and $CdSO_4 \cdot 8/3\ H_2O$ (0.10 mmol, 25.6 mg) disolved in ethanol (3 mL) and H_2O (3 mL) was

***Corresponding author: Gaoyuan Xu,** Department of Social Science, Henan Polytechnic University, Jiaozuo 454000, P. R. China, e-mail: lihuijunxgy@hpu.edu.cn
Ning Zhang, Meijie Su and Huijun Li: College of Chemistry and Chemical Engineering, Henan Polytechnic University, Jiaozuo 454000, P. R. China

Table 1: Data collection and handling.

Crystal:	Yellow block
Size:	0.30 × 0.20 × 0.20 mm
Wavelength:	Mo *Kα* radiation (0.71073 Å)
μ:	0.83 mm^{-1}
Diffractometer, scan mode:	Bruker SMART APEX CCD, ω
θ_{max}, completeness:	25.0°, 97%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	7050, 2474, 0.017
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2307
$N(param)_{refined}$:	189
Programs:	SHELX [2], Bruker [3]

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.5000	0.41214(2)	0.2500	0.03854(11)
O1	0.38337(14)	0.48816(11)	0.13097(15)	0.0493(5)
N1	0.61917(17)	0.31227(14)	0.23706(19)	0.0483(5)
N2	0.7502(2)	0.20581(18)	0.1971(3)	0.0715(8)
N3	0.48666(14)	0.38403(12)	0.06279(17)	0.0353(4)
N4	0.41315(15)	0.42105(12)	−0.02201(18)	0.0379(5)
N5	0.1476(2)	0.60124(17)	−0.0934(2)	0.0632(7)
C1	0.6858(2)	0.2756(2)	0.3227(3)	0.0645(9)
H1	0.6891	0.2864	0.3989	0.077*
C2	0.7499(3)	0.2223(2)	0.3024(3)	0.0718(10)
H2	0.7946	0.1971	0.3651	0.086*
C3	0.6838(2)	0.24277(19)	0.1114(3)	0.0576(7)
H3	0.6818	0.2321	0.0356	0.069*
C4	0.61728(18)	0.29628(15)	0.1287(2)	0.0402(6)
C5	0.54229(17)	0.33583(15)	0.0320(2)	0.0384(5)
C6	0.5351(2)	0.3194(2)	−0.0914(2)	0.0549(7)
H6A	0.4808	0.3479	−0.1422	0.082*
H6B	0.5262	0.2632	−0.1064	0.082*
H6C	0.5938	0.3364	−0.1048	0.082*
C7	0.36656(17)	0.47196(14)	0.0246(2)	0.0361(5)
C8	0.28466(17)	0.51397(14)	−0.0613(2)	0.0369(5)
C9	0.2676(2)	0.50925(18)	−0.1795(2)	0.0476(6)
H9	0.3070	0.4778	−0.2091	0.057*
C10	0.1919(2)	0.5515(2)	−0.2525(3)	0.0586(8)
H10	0.1796	0.5497	−0.3324	0.070*
C11	0.1345(2)	0.5965(2)	−0.2065(3)	0.0627(9)
H11	0.0837	0.6253	−0.2570	0.075*
C12	0.2225(2)	0.56106(18)	−0.0233(3)	0.0503(7)
H12	0.2339	0.5649	0.0563	0.060*

Table 2 (continued)

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
O2	0.4784(3)	0.1325(3)	−0.0114(4)	0.1442(15)
H2A	0.5123	0.1045	−0.0384	0.216*
C13	0.4802(5)	0.1030(4)	0.0939(6)	0.134(2)
H13A	0.5333	0.1265	0.1538	0.201*
H13B	0.4884	0.0462	0.0946	0.201*
H13C	0.4201	0.1156	0.1073	0.201*

placed in a glass bottle (10 mL) at room temperature. Yellow block crystals were obtained after 3 days.

Experimental details

The structure was solved by Direct Methods and refined with the SHELX crystallographic software package [2, 3]. The hydrogen atoms were placed at calculated positions and refined as riding atoms with isotropic displacement parameters.

Comment

Hydrazones are a class of compounds which are well known for their antimicrobial activity [4, 5]. But as hydrazones are prone to undergo degradation and bacteria can develop resistance to them, complexation of hydrazones with biocompatible metal ions is useful in this regard for long-term effectiveness [6]. In the course of our studies on the chemistry of lanthanide compounds, we have prepared and characterized a number of hydrazone ligands. Herein we report a new Cd(II) complex derived from (*E*)-*N*′-(1-(pyrazin-2-yl) ethylidene)nicotinohydrazide (HL).

The title complex is a mononuclear coordination compound in which the six-coordinated Cd^{2+} is surrounded by two acylhydrazones. Each ligand provides a ON2 donor set thus giving distorted octahedral geometry. The bond lengths of Zn—O and Zn—N (2.0670(19)–2.198(2) Å) in the title complex are comparable with those found in our previous work [7]. In the solid state, the lattice ethanol molecule is linked to the mononuclear coordinational compound by an intermolecular N—H···O hydrogen bond.

References

1. Das, L. K.; Diaz, C.; Ghosh. A.: Antiferromagnetic mixed-valence Cu two-dimensional coordination polymers constructed by double oximato bridged Cu dimers and CuISCN based one-dimensional anionic chains. Cryst. Growth Des. **15** (2017) 3939–3949.
2. Sheldrick, G. M.: Crystal refinement with *SHELX*. Acta Crystallogr. **C71** (2015) 3–8.
3. Bruker. *SMART* and *SAINT*. Bruker AXS Inc., Madison, WI, USA (2007).
4. Liu, Y.-F.; Liu, Y.-P.; Zhang, K.-K.; Ren, Q.-L.; Qin, J.: Mononuclear and three-dimensional metal complexes based on a multidentate hydrazone ligand. Acta Crystallogr. **C71** (2015) 116–121.
5. Yan, L.-L.; Cai, H.-X.: Crystal structure of 3-benzyl-2,3-dihydro-2-thioxoquinazolin-4(1*H*)-one. Z. Kristallogr. NCS **232** (2017) 811–812.
6. Bakale, R. P.; Pathan, A. H.; Naik, G. N.; Machakanur, S. S.; Mangannavar, C. V.; Muchchandi, I. S.; Gudasi, K. B.: Synthesis and characterization of transition metal complexes of hydrochloride salt of 3-chlorobenzaldehyde hydralazine hydrazone: a new class of possible anti-cariogenic agents. Appl. Organomet. Chem. **28** (2014) 720–724.
7. Xu, Z.-Q.; Mao, X.-J.; Jia, L.; Xu, J.; Zhu, T.-F.; Cai, H.-X.; Bie, H.-Y.; Chen,R.-H.; Ma, T.-l.: Synthesis, characterization and anticancer activities of two lanthanide(III) complexes with a nicotinohydrazone ligand. J. Mol. Struct. **1102** (2015) 86–90.