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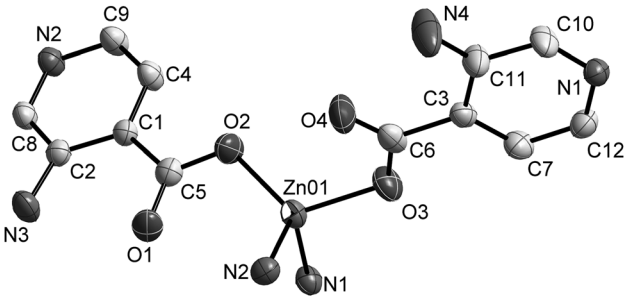
The crystal structure of poly [bis(μ_2–3–*aminopyridine*–4–*carboxylato*–κ^2N:*O*) Zinc(II)], $[Zn(C_6H_5N_2O_2)_2]_n$



https://doi.org/10.1515/ncrs-2023-0358
Received August 2, 2023; accepted September 5, 2023;
published online September 19, 2023

Abstract

$[Zn(C_6H_5N_2O_2)_2]_n$, orthorhombic, $P2_12_12_1$ (no. 19), a = 7.6139(7) Å, b = 12.4890(13) Å, c = 13.9382(13) Å, V = 1325.4(2) Å^3, Z = 4, $R_{gt}(F)$ = 0.0391, $wR_{ref}(F^2)$ = 0.0710, T = 296 K.

CCDC no.: 2285875

Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

1 Source of materials

A mixture of $Zn(NO_3)_2{\cdot}6H_2O$ (0.1 mmol 0.030 g), 3-aminoisonicotinic acid (0.4 mmol 0.055 g), H_2O (8 mL) was sealed in a 25-mL Teflon-lined steel autoclave, and heated at 453 K for 10 days, then slowly cooled to room temperature. Yellow block crystals of title complex could be seen in the product.

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Table 1: Data collection and handling.

Crystal:	Yellow block
Size:	0.18 × 0.15 × 0.15 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	1.88 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max}, completeness:	27.6°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	8073, 3023, 0.046
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 2424
$N(param)_{refined}$:	191
Programs:	Bruker [1], Diamond [2], Olex2 [3], SHELX [4, 5]

2 Experimental details

All hydrogen atoms were placed in calculated positions and refined as riding atoms. The values were set to be 1.2 U_{eq} of the parent atoms.

3 Comment

The complexes of isonicotinic acid and its derivatives have attracted a lot of attentions [6–10]. However, coordination of 3-aminoisonicotinic acid has been less studied. A complex ($[Zn(C_6H_5N_2O_2)_2]_n$) of 3-aminoisonicotinic acid has been prepared under hydrothermal reaction conditions. The asymmetric unit of title complex contains one Zn^{2+} ion and two L^- anions (HL = 3-aminoisonicotinic acid). Each Zn(II) ion has a distorted tetrahedron coordination (see the figure), formed by two carboxylate oxygen atoms and two pyridyl nitrogen atoms of four different bridging L^- ligands. The Zn–O distances are nearly equivalent spanning a narrow range of 1.950(3)–1.953(3) Å, and the Zn–N distances vary from 2.027(4) to 2.061(4) Å [11–13]. The N–Zn–O angles are in the range 98.53(15)–119.14(16)°, the N–Zn–N angle is 107.28(15)°, and the O–Zn–O angle is 117.19(15)°. All L^- ligands act as μ_2-bridges, linking two Zn(II) ions.

Each Zn(II) ions is connected to four adjacent Zn(II) ions via four μ_2 L^- ligands, forming the 3–D polymeric structure of the title complex. Identical adamantanoid cages can be found in the structure. In the cages, the Zn–Zn edges are

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Zn01	0.40340 (6)	0.55320 (4)	0.72064 (4)	0.02899 (15)
O1	0.2312 (5)	0.6572 (3)	0.8818 (2)	0.0409 (9)
O2	0.2883 (4)	0.6927 (2)	0.7283 (3)	0.0404 (8)
O3	0.5196 (5)	0.5171 (3)	0.6003 (3)	0.0447 (10)
N1	0.9465 (5)	0.4970 (3)	0.3320 (3)	0.0294 (10)
O4	0.6962 (5)	0.6497 (3)	0.6392 (3)	0.0545 (11)
N2	−0.1933 (4)	0.9498 (3)	0.7895 (3)	0.0314 (8)
N3	−0.0059 (6)	0.7805 (3)	0.9737 (3)	0.0405 (11)
H3A	−0.073203	0.799180	1.020349	0.049*
H3B	0.075379	0.733814	0.982894	0.049*
C1	0.0739 (6)	0.7973 (3)	0.8055 (3)	0.0249 (10)
C2	−0.0277 (6)	0.8248 (4)	0.8858 (3)	0.0268 (11)
C3	0.7595 (6)	0.5489 (5)	0.4982 (3)	0.0297 (10)
C4	0.0406 (5)	0.8518 (4)	0.7211 (4)	0.0327 (10)
H4	0.109485	0.837361	0.667545	0.039*
C5	0.2073 (6)	0.7102 (4)	0.8071 (3)	0.0296 (11)
C6	0.6543 (7)	0.5755 (5)	0.5859 (4)	0.0359 (13)
C7	0.7158 (7)	0.4618 (4)	0.4418 (3)	0.0362 (12)
H7	0.621118	0.419031	0.459420	0.043*
C8	−0.1603 (6)	0.9004 (4)	0.8724 (3)	0.0307 (12)
H8	−0.230379	0.917560	0.924867	0.037*
C9	−0.0902 (6)	0.9264 (3)	0.7138 (3)	0.0355 (11)
H9	−0.108348	0.961438	0.655730	0.043*
C10	0.9884 (7)	0.5818 (4)	0.3831 (4)	0.0424 (14)
H10	1.080351	0.624565	0.361673	0.051*
C11	0.9015 (8)	0.6114 (4)	0.4684 (3)	0.0444 (13)
C12	0.8088 (6)	0.4369 (4)	0.3607 (3)	0.0366 (12)
H12	0.776369	0.377456	0.324578	0.044*
N4	0.9611 (8)	0.6992 (4)	0.5176 (4)	0.106 (3)
H4A	0.983279	0.749859	0.477434	0.127*
H4B	0.879417	0.719749	0.556284	0.127*

8.7976(9) or 8.8427(9) Å long, the Zn–Zn–Zn angles vary between 90.437(6) and 126.638(7)°, and the maximal dimensions of the cage is 22.8417(22) Å. Large cavities can be found in the structure of title complex, inducing 3-fold interpenetration of the networks. The separated distances from one net to other interpenetrating one is 7.6139(10) Å.

Research ethics: Not applicable.

Author contributions: The authors have accepted responsibility for the entire content of this manuscript and approved its submission.

Competing interests: The authors state no conflict of interest.

Research funding: NSF (Natural Science Foundation) of Anhui Province (2108085MB53), the NSF for Distinguished Young Scholars of Anhui University (2022AH020087), University NSF of Anhui Province (KJ2020A0647), Research Program of Huainan Normal University (2020XJYB003), Project of Huainan City and Program for Innovation Research Team in Huainan Normal University (XJTD202006).

Data availability: The raw data can be obtained on request from the corresponding author.

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