APPLIED ORGANOMETALLIC CHEMISTRY
Appl. Organometal. Chem. 2005; **19**: 189–190
Main Group Metal Compounds
Published online in Wiley InterScience (www.interscience.wiley.com). DOI:10.1002/aoc.772

Crystallographic report

Polymeric [diaqua bis(3-pyridylacrylato)zinc(II)]

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Received 9 July 2004; Revised 26 July 2004; Accepted 27 July 2004

The Zn center in [bis(3-pyridylacrylato)diaquazinc(II)]$_n$ is in a slightly distorted octahedral geometry within a *cis*-N_2O_4 donor set. Each tridentate 3-pyridylacrylate ligand links two Zn centers, resulting in the formation of a linear chain. Copyright © 2004 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; hydrothermal synthesis; zinc complex

COMMENT

The local coordination geometry around Zn center in $[Zn(3\text{-}C_5H_4N{-}CH{=}CHCO_2)_2(OH_2)_2]_n$ is a slightly distorted octahedron defined by two water molecules, two O atoms of one tridentate 3-pyridylacrylate, which links a translationally related Zn atom via its N atom, and an N atom of a second 3-pyridylacrylate ligand (the carboxylate ligand does not bridge in this case) as shown in Fig. 1. A one-dimensional infinite chain results, in contrast to that found in Zn[(*E*)-3-$C_5H_4N{-}CH{=}CH{-}COO$](OH).[1] The chains are linked, via H bonds, into a layer structure.

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Contract/grant sponsor: Distinguished Young Scholar Fund; Contract/grant number: 20225103.
Contract/grant sponsor: Specialized Research Fund for the Doctoral Program of Higher Education; Contract/grant number: 20030284001.

EXPERIMENTAL

Hydrothermal treatment of $Zn(ClO_4)_2{\cdot}6H_2O$ (0.4 mmol), racemic 3-pyridyl-3-aminopropionic acid (0.2 mmol), water (3.0 ml) and 2-butanol (14.0 ml) over 2 days at 160 °C yielded crystalline colorless needles. The yield was about 35% based on the carboxylic acid. Intensity data were collected at 293(2) K on a Bruker AXS SMART CCD for a colorless block $0.10 \times 0.20 \times 0.50$ mm^3. $C_{16}H_{16}N_2O_6Zn$, $M = 397.68$, triclinic, *Pbar*1, $a = 7.6337(4)$, $b = 9.6381(5)$, $c = 11.9809(6)$ Å, $\alpha = 66.976(1)$, $\beta = 81.329(1)$, $\gamma = 84.923(1)°$, $V = 801.57(7)$ Å^3, $Z = 2$, 3127 unique data ($\theta_{max} = 26.0°$), $R = 0.035$ (2932 [$I \geq 2\sigma(I)$] reflections), $wR = 0.117$ (all data). Programs used: SAINT, SADABS, SHELX-97 and ORTEP. CCDC deposition no. 237536.

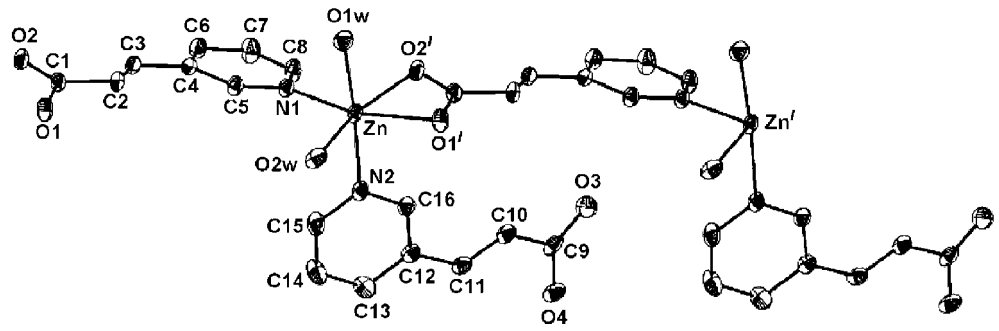

Figure 1. Molecular structure of $[Zn(3\text{-}C_5H_4N{-}CH{=}CHCO_2)_2(OH_2)_2]_n$; H atoms are omitted for clarity. Selected geometric parameters: Zn–O1^i 2.1162(18), Zn-O1w 2.1431(19), Zn-O2w 1.9985(18), Zn–O2^i 2.2496 (18), Zn-N1 2.101(2), Zn-N2 2.242(2) Å; O1^i–Zn–O2^i 60.28(7), O1w-Zn-O2w 89.48(8), O1w-Zn-N1 88.54(8), O1w-Zn-N2 176.06(7), O2w-Zn-N1 100.13(8), O2w-Zn-O1^i 105.65(8)°. Symmetry operation *i*: x, $-1 + y$, z.

Acknowledgements

This work was supported by the Distinguished Young Scholar Fund, to R.-G. Xiong (no. 20225103), and the Specialized Research Fund for the Doctoral Program of Higher Education (no. 20030284001).

REFERENCE

1. Qu ZR, Zhao H, Wang YP, Wang XS, Ye Q, Li YH, Xiong RG, Abrahams BF, Liu ZG, You XZ. *Chem. Eur. J.* 2004; **10**: 53.