APPLIED ORGANOMETALLIC CHEMISTRY
Appl. Organometal. Chem. 2005; **19**: 393
Main Group Metal Compounds
Published online in Wiley InterScience (www.interscience.wiley.com). DOI:10.1002/aoc.775

Crystallographic report

Chloro[1,3-bis[2-[2-[(4-methoxybenzyl) amino]ethylamino]]-2-propanol]zinc(II) chloride hydrate, $[(C_{23}H_{36}N_4O_3)ZnCl]Cl\cdot H_2O$

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Received 13 January 2004; Accepted 26 January 2004

The zinc(II) center in the molecule of $[(C_{23}H_{36}N_4O_3)ZnCl]Cl\cdot H_2O$ is coordinated by four nitrogen atoms of HL (1,3-bis[2-[2-[(4-methoxybenzyl) amino]ethylamino]]-2-propanol) and one chloro anion. The coordination moieties are connected by hydrogen bonds to form a one-dimensional structure.

KEYWORDS: crystal structure; zinc complex; one-dimensional structure; 1,3-bis[2-[2-[(4-methoxybenzyl) amino]ethylamino]]-2-propanol

COMMENT

The coordination geometry of mononuclear zinc complex $[(C_{23}H_{36}N_4O_3)ZnCl]Cl\cdot H_2O$ (**1**) is square pyramidal (Fig. 1). The zinc(II) center is coordinated by one chloro anion and four nitrogen atoms from HL. The Zn–N distances are in the normal range.[1] It is interesting that noncoordinated chlorides form multiple hydrogen bonds with crystal lattice water molecules and N–H and O–H donor sets of HL, resulting in a one-dimensional structure along the *b* axis (Fig. 1).

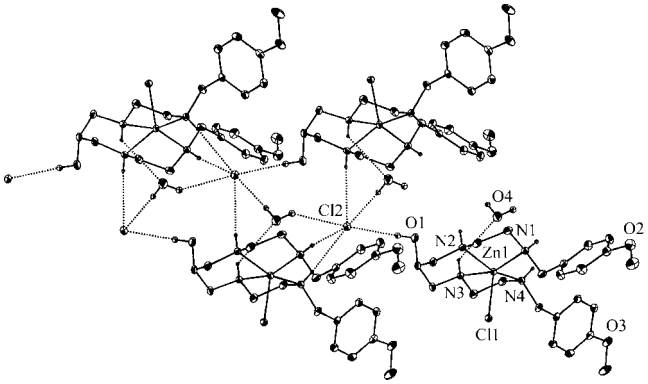

Figure 1. One-dimensional structure of **1**.

EXPERIMENTAL

Synthesis of HL·4HCl: the reaction of epichlorohydrin with excessive ethylenediamine yielded a light yellow intermediate, which was used to react with 4-methoxybenzaldehyde by the method reported[2] to give HL·4HCl. Anal. Found: C, 49.40; H, 7.07; N, 9.84. Calc. for $C_{23}H_{40}N_4O_3Cl_4$: C, 49.12; H, 7.17; N, 9.96%.

1 was synthesized by the reaction of $Zn(ClO_4)\cdot 6H_2O$, HL·4HCl and NaOH (molar ratio, 1 : 1 : 4) in methanol. The concentrated solution was left for slow evaporation of the solvent to give colorless crystals. Anal. Found: C, 48.21; H, 6.85; N, 9.61. Calc. for $C_{23}H_{38}Cl_2N_4O_4Zn$: C, 48.39; H, 6.71; N, 9.82%.

Intensity data were collected at 291 K on a Rigaku RAXIS-IV diffractometer for a colorless crystal $0.20 \times 0.18 \times 0.18$ mm^3. $C_{23}H_{38}Cl_2N_4O_4Zn$, $M = 570.84$, monoclinic, $P21/n$, $a = 11.527(2)$, $b = 10.133(2)$, $c = 23.034(5)$ Å, $\beta = 95.51(3)°$, $V = 2678.1(9)$ Å^3, $Z = 4$, 4223 unique data (θ_{max} 25.00°), 3439 data with $I > 2\sigma(I)$, $R_1 = 0.0274$, $wR_2 = 0.0486$ [$I > 2\sigma(I)$], $R_1 = 0.0495$, $wR_2 = 0.0514$ (all data), $\rho_{max} = 0.193$ e$^-$ Å^{-3}. Programs used: SHELXS-97, SHELXL-97. CCDC deposition number: 224 209.

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Contract/grant sponsor: National Natural Science Foundation of China; Contract/grant number: 30270321.

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