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Key indicators

Single-crystal X-ray study
T = 234 K
Mean $\sigma(\text{C}-\text{C}) = 0.006 \text{ \AA}$
R factor = 0.041
wR factor = 0.127
Data-to-parameter ratio = 18.4

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

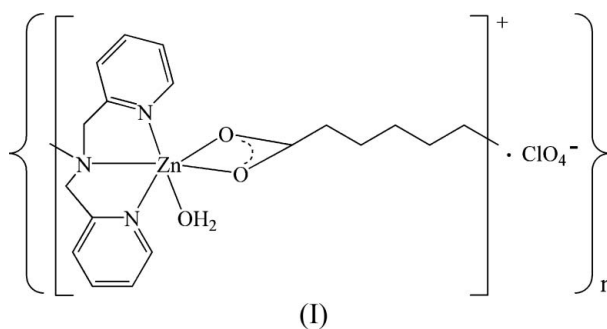
catena-Poly[[[aquazinc(II)]- μ -6-[bis(2-pyridylmethyl)amino]caproato] perchlorate]

The tetradentate Schiff base carboxylate-containing ligand bis(2-pyridylmethyl)amino-6-caproic acid (Hpmca) reacts with zinc(II) perchlorate to give the title one-dimensional zinc(II) complex, $\{[\text{Zn}(\text{C}_{18}\text{H}_{22}\text{N}_3\text{O}_2)(\text{H}_2\text{O})](\text{ClO}_4)_n$ or $\{[\text{Zn}(\mu\text{-pmca})(\text{H}_2\text{O})](\text{ClO}_4)_n$. Each Zn^{II} ion has a distorted octahedral geometry, being coordinated by three N atoms of the ligand, two O atoms belonging to another ligand, and one water molecule.

Received 5 October 2005
Accepted 27 October 2005
Online 5 November 2005

Comment

The Schiff base carboxylate-containing ligand bis(2-pyridylmethyl)amino-3-propionic acid (Hpmpa) reacts with copper(II) perchlorate to give the one-dimensional chain complex $\{[\text{Cu}(\mu\text{-pmpa})](\text{ClO}_4)_2\text{H}_2\text{O}\}_n$ (Choi, Jeon, Ryu *et al.*, 2004). However, the reaction of Hpmpa with CuCl_2 leads to the mononuclear complex $[\text{Cu}(\text{Hpmpa})\text{Cl}]\text{Cl}\cdot 2\text{H}_2\text{O}$, in which the Cu^{II} ion exhibits a square-pyramidal coordination environment with the three N atoms and the carboxylate O atom of the ligand and one Cl^- anion (Choi, Jeon, Lee *et al.*, 2004). In this case, the Cl^- ligands remain coordinated to the Cu^{II} ion, thus preventing a self-assembly reaction through the carboxylate group. In order to better understand some aspects of different molecular topologies, we prepared the title one-dimensional zinc(II) complex, $\{[\text{Zn}(\mu\text{-pmca})(\text{H}_2\text{O})](\text{ClO}_4)_n$, (I), and present its structure here.



Because the ligand does not saturate the coordination positions on the Zn^{II} ion, a self-assembly reaction may occur through the deprotonated carboxylate group, leading to a ligand-bridged one-dimensional chain with an intramolecular $\text{Zn}\cdots\text{Zn}$ distance of $9.745(3) \text{ \AA}$. Each Zn^{II} ion is in a distorted octahedral geometry, being coordinated by three N atoms of the ligand, two O atoms of another ligand, and one water molecule. The carboxylate group adopts a bidentate chelating mode [$\text{Zn}-\text{O}1 = 2.098(2) \text{ \AA}$, $\text{Zn}-\text{O}2 = 2.285(3) \text{ \AA}$ and $\text{O}1-$

Zn—O2 = 59.39 (8)°; Table 1]. The Zn—OW1 distance of 2.110 (3) Å is in the normal range, as found in a related coordination complex (Choi & Jeon, 2003). The Zn—N2 (tertiary amine) distance of 2.187 (3) Å is slightly longer than the secondary Zn—N1 and Zn—N3 distances [(2.094 (3) and 2.082 (3) Å, respectively]. The N1—Zn—N2 and N2—Zn—N3 bite angles of the five-membered chelate rings are 79.74 (11) and 80.98 (12)°, respectively. The average N2—C distance [1.489 (3) Å] involving the tertiary amine is approximately 0.15 Å longer than the average N1—C [1.341 (4) Å] and N3—C [1.330 (3) Å] distances involving the secondary amines. This fact may be due to the sp^3 -hybridization of the coordinated tertiary N atom.

As shown in Table 2, the coordinated water molecule forms hydrogen bonds with the carboxylate and perchlorate O atoms.

Experimental

Bis(2-pyridylmethyl)amino-6-caproic acid (Hpmca) was prepared in the following manner. To an aqueous solution (25 ml) of 2-picoyl chloride hydrochloride (3.61 g, 22 mmol) was added an aqueous solution (25 ml) of 6-aminocaproic acid (1.31 g, 10 mmol) and NaOH (1.6 g, 40 mmol). After heating the mixture to reflux for 1 d, the solution was extracted with chloroform. Removal of the solvent yielded a crude white product, which was purified by recrystallization from a hot H₂O—MeOH solution (1:1, 30 ml). Crystals of the title compound, (I), were isolated as colourless blocks from the attempted reaction of Hpmca (136 mg, 0.5 mmol) and Zn(ClO₄)₂·6H₂O (186 mg, 0.5 mmol) in an aqueous medium. The product was recrystallized from a hot H₂O—MeCN solution (1:1, 10 ml).

Crystal data

[Zn(C ₁₈ H ₂₂ N ₃ O ₂)(H ₂ O)](ClO ₄)	Mo K α radiation
$M_r = 495.22$	Cell parameters from 4492 reflections
Orthorhombic, <i>Pbca</i>	$\theta = 2.6\text{--}23.1^\circ$
$a = 15.9996$ (7) Å	$\mu = 1.37$ mm ⁻¹
$b = 15.3187$ (6) Å	$T = 233.5$ (2) K
$c = 16.7417$ (7) Å	Block, colourless
$V = 4103.3$ (3) Å ³	0.31 × 0.18 × 0.13 mm
$Z = 8$	
$D_x = 1.603$ Mg m ⁻³	

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	5109 independent reflections
ω scans	3087 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan <i>SADABS</i> (Sheldrick, 1996)	$R_{\text{int}} = 0.055$
$T_{\text{min}} = 0.646$, $T_{\text{max}} = 0.840$	$\theta_{\text{max}} = 28.3^\circ$
28748 measured reflections	$h = -21 \rightarrow 19$
	$k = -20 \rightarrow 12$
	$l = -21 \rightarrow 22$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0446P)^2 + 6.9671P]$
$R[F^2 > 2\sigma(F^2)] = 0.041$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.127$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.03$	$\Delta\rho_{\text{max}} = 0.55$ e Å ⁻³
5109 reflections	$\Delta\rho_{\text{min}} = -0.39$ e Å ⁻³
277 parameters	
H atoms treated by a mixture of independent and constrained refinement	

Table 1
Selected geometric parameters (Å, °).

Zn—N3	2.082 (3)	O1—C13	1.274 (4)
Zn—N1	2.094 (3)	O2—C13	1.242 (4)
Zn—O1	2.098 (2)	N1—C1	1.329 (5)
Zn—OW1	2.110 (3)	N1—C5	1.352 (5)
Zn—N2	2.187 (3)	N2—C18	1.481 (4)
Zn—O2	2.285 (3)	N2—C7	1.481 (5)
Cl1—O4	1.397 (4)	N2—C6	1.506 (5)
Cl1—O6	1.409 (3)	N3—C12	1.326 (5)
Cl1—O3	1.414 (4)	N3—C8	1.334 (4)
Cl1—O5	1.425 (4)	C13—C14	1.507 (5)
N3—Zn—N1	159.26 (12)	O6—Cl1—O3	108.1 (3)
N3—Zn—O1	101.18 (11)	O4—Cl1—O5	112.0 (3)
N1—Zn—O1	99.10 (11)	O6—Cl1—O5	109.4 (3)
N3—Zn—OW1	87.66 (12)	O3—Cl1—O5	108.5 (3)
N1—Zn—OW1	85.17 (12)	C1—N1—C5	117.8 (3)
O1—Zn—OW1	98.44 (10)	C1—N1—Zn	127.5 (3)
N3—Zn—N2	80.98 (12)	C5—N1—Zn	113.6 (3)
N1—Zn—N2	79.74 (11)	C18—N2—C7	111.7 (3)
O1—Zn—N2	170.28 (10)	C18—N2—C6	107.4 (3)
OW1—Zn—N2	91.09 (11)	C7—N2—C6	112.0 (3)
N3—Zn—O2	90.97 (11)	C12—N3—C8	119.5 (3)
N1—Zn—O2	103.08 (11)	C12—N3—Zn	125.9 (2)
O1—Zn—O2	59.39 (8)	C8—N3—Zn	114.6 (3)
OW1—Zn—O2	157.07 (10)	O2—C13—O1	119.8 (3)
N2—Zn—O2	111.30 (9)	O2—C13—C14	120.7 (3)
O4—Cl1—O6	109.0 (3)	O1—C13—C14	119.5 (3)
O4—Cl1—O3	109.8 (3)		

Table 2
Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
OW1—H19 <i>A</i> ...O1 ⁱ	0.74 (4)	1.95 (5)	2.683 (4)	175 (5)
OW1—H19 <i>B</i> ...O6 ⁱ	0.80 (5)	2.02 (5)	2.817 (5)	171 (4)

Symmetry code: (i) $-x, -y + 1, -z + 1$.

The two H atoms of the water molecule were found in a difference Fourier map and their positions were refined, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{OW1})$. Other H atoms were placed in calculated positions, with C—H = 0.93–0.97 Å, and allowed to ride on their parent C atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT-Plus* (Bruker, 1999); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

This work was supported by a grant (No. R05–2003–000–10536–0) from the Basic Research Programme of the Korea Science and Engineering Foundation.

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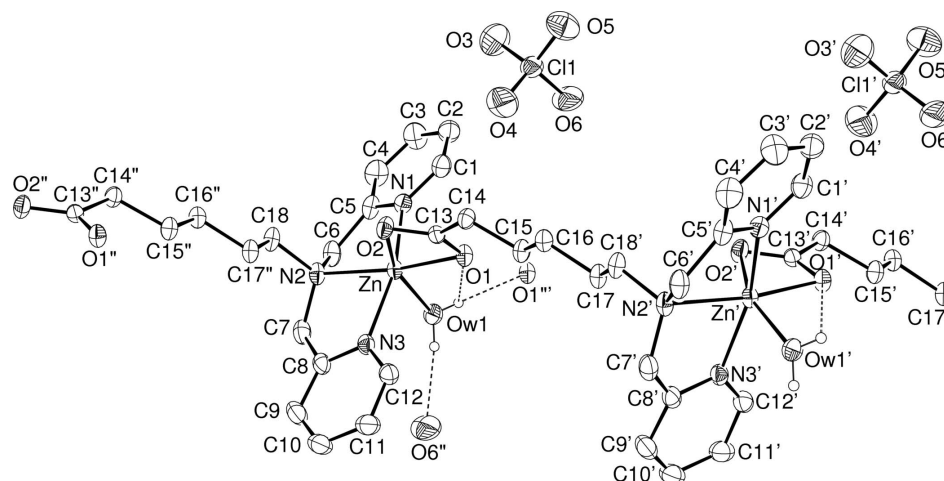


Figure 1

A diagram showing the one-dimensional chain of (I). Unprimed atoms are in the asymmetric unit and primed atoms are obtained by *c*-glide planes parallel to [010]. H atoms have been omitted for clarity.

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