C13—C8—N2	119.6 (9)	C18—N3—C14	117.6 (11)
C10—C9—C8	117.6 (11)	C16—C15—C14	115.8 (13)
C12—C11—C10	120.3 (14)	C18—C17—C16	116.9 (13)
C12—C13—C8	122.1 (11)	C19—C18—N3	113.8 (10)
C15—C14—N3	123.8 (12)	C23—N4—C19	123.5 (10)
C17—C16—C15	122.8 (14)	C42—C41—C40	118.9 (14)
C17—C18—N3	122.9 (11)	C43—C42—C41	118.8 (14)
C19—C18—C17	123.3 (11)	C42—C43—N8	122.9 (12)
N4—C19—C18	112.1 (10)	C22—C21—C20	121.6 (12)
C20—C19—C18	127.3 (11)	C22—C23—N4	116.3 (10)
C20—C19—N4	120.5 (11)	C24—C23—C22	131.8 (11)
C21—C20—C19	117.8 (12)	N5—C24—C23	118.5 (10)
C23—C22—C21	120.1 (12)	C25—C24—N5	118.5 (11)
C24—C23—N4	111.9 (10)	C27—C26—C25	122.5 (14)
C28—N5—C24	121.4 (10)	C27—C28—N5	121.8 (12)
C25—C24—C23	123.0 (11)	C30—C29—N6	121.6 (13)
C26—C25—C24	118.8 (13)	C32—C31—C30	119.2 (15)
C28—C27—C26	117.0 (13)	C32—C33—N6	117.7 (11)
C33—N6—C29	119.9 (11)	C34—C33—C32	124.8 (12)
C31—C30—C29	121.2 (15)	N7—C34—C33	112.3 (10)
C33—C32—C31	120.3 (13)	C35—C34—N7	118.2 (11)
C34—C33—N6	117.5 (11)	C37—C36—C35	122.0 (13)
C38—N7—C34	122.8 (9)	C37—C38—N7	121.7 (10)
C35—C34—C33	129.5 (11)	C39—C38—C37	125.8 (10)
C36—C35—C34	119.3 (12)	N8—C39—C38	115.7 (10)
C38—C37—C36	116.0 (12)	C40—C39—N8	117.5 (11)
C39—C38—N7	112.6 (9)		

An empirical absorption correction based on ψ scans of six reflections was used. The goodness of fit for merging in point group *mm*2 was 1.35 (two data sets were collected within the stated octants; $R_{\rm merge}$ for 165 reflections with exactly two observations, 0.008). Attempted merging of the data in point group *mmm* gave a goodness of fit of only 2.0, and the molecular symmetry could not be satisfied by the centrosymmetric equivalent of the space group (*Pnma*). All reflections were used in solution and refinement of the structure. Coordinates of the Pt atoms were found from a Patterson map, the remaining heavy atoms (including a water molecule of crystallization and three perchlorate ions) were found by successive structure factor-Fourier calculations. F_o^2 magnitudes were used in full-matrix least-squares refinement, which minimized $\Sigma w(F_o^2 - F_c^2)$; *R* based on *F*; *wR* based on F^2; H atoms were positioned by calculation (C—H, 0.95 Å) and included as constant contributions to the structure factors (except H atoms on the water molecule, which were ignored). Hydrogen parameters were not refined but repositioned twice near the end of the refinement. The weights were taken as $1/\sigma^2(F_o^2)$; variances $[\sigma^2(F_o^2)]$ derived from counting statistics plus an additional term, $(0.014I)^2$; variances of the merged data by propagation of error plus an additional term $(0.014\bar{I})^2$. Atomic scattering factors and values for $\Delta f'$ taken from Cromer & Waber (1974) and Cromer (1974); programs used were those from the *CRYM* crystallographic computing system (Duchamp, 1964) and *ORTEP* (Johnson, 1976). Final atomic coordinates and $U_{\rm eq}$ values are listed in Table 1 with selected distances and angles given in Table 2. The data were averaged in point group *mm*2 for final refinement. Refinement with f'' positive gave significantly poorer *R* indices and goodness of fit than with f'' negative. A background correction derived from the backgrounds of weak reflections as a function of 2θ was applied to all reflections.

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Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and complete geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55628 (27 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: SP1005]

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Structure of [1,9-Bis(2-pyridyl)-2,5,8-triazanonane]zinc(II) Tetrachlorozincate(II)

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Abstract

The cationic complex is five coordinated and shows a distorted geometry intermediate between a square-based pyramid and a trigonal bipyramid. Not all the Zn—N distances are equivalent. The $ZnCl_4^{2-}$ anion shows a tetrahedral geometry.

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Comment

It has been proposed that pentacoordinated zinc centres are present in catalytic reaction intermediates of enzymes (Bertini & Luchinat, 1983) and may therefore be essential for their catalytic function. However, although this has prompted the synthesis and study of several pentacoordinated zinc complexes (Solá, Lledós, Durán & Bertrán, 1991; Kimura, Koike & Toriumi, 1988), there are not many complexes that are structurally well characterized.

Linear polydentate ligands have the possibility of forming a wide range of isomers, both geometrical and conformational, and can therefore provide a series of compounds in which to study some of the factors that affect the stability and reactivity of a particular complex.

Several complexes of the ligand 1,9-bis(2-pyridyl)-2,5,8-triazanonane (picdien) have been prepared and their X-ray crystal structures determined (Raleigh & Martell, 1985; Ahmed, Chatterjee, Cooksey, Tobe, Williams & Humanes, 1989; Ugalde-Saldívar, Luna-Canut, Sosa-Torres, Rosales-Hoz, Toscano & Tobe, 1990). In all these cases, the ligand was found to be pentacoordinated. It was interesting therefore to prepare the zinc derivative of this ligand and determine its structure. The results of this study are reported herein. The title compound was synthesized by dissolving picdien (1.0395 g) in 30 ml of ethanol and adding a solution of $ZnCl_2$ in 45 ml of ethanol. The final solution was warmed and evaporated whilst being stirred until two thirds of the initial volume, at which point the compound started to crystallize out. The solid was filtered off, washed with cold ethanol and air-dried (0.4160 g). The crystals were grown by slow evaporation of the solution of the compound. (Found: C, 34.39; H, 4.15; N, 12.38. $C_{16}H_{23}N_5Cl_4Zn_2$ requires C, 34.44; H, 4.15; N, 12.55%.)

Final positional parameters are listed in Table 1 and bond lengths and bond angles are given in Table 2. A molecular diagram including the numbering scheme is shown in Fig. 1. The compound is formed by discrete $[Zn(picdien)]^{2+}$ cations and $[ZnCl_4]^{2-}$ anions. The cation is a five-coordinated complex in which all the N atoms are bonded to the Zn atom. The geometry could be described as a distorted trigonal bipyramid. The N(1)—Zn—N(4) angle is 174.7 (2)°, so N(1) and N(4) could be said to be occupying the axial positions of the bipyramidal arrangement. The sum of the angles formed by N(2), N(3) and N(5) about the Zn atom is 354.8°, but there are large differences between the angles, N(2)—Zn—N(3), N(2)—Zn—N(5) and N(3)—Zn—N(5) having values of 82.7 (2), 117.2 (2) and 154.9 (2)°. Even though Zn^{II} is a d^{10} ion and no differences are expected between the apical and equatorial bond lengths, significant differences have been reported for other complexes (Kimura, Koike & Toriumi, 1988; Ray & Hathaway, 1980). The N(2) and N(4) bonds to the Zn ion are the longest in the compound, but the differences between N(4)—Zn and the remaining Zn—N bonds are not significant. All the Zn—N distances are similar to those previously reported (Andreetti, Jain & Lingafelter, 1969; Goedken & Christoph, 1973).

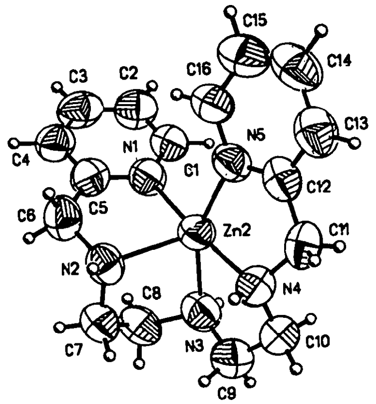

Fig. 1. *ORTEP* (Johnson, 1965) diagram of the $[Zn(picdien)]^{2+}$ cation with thermal ellipsoids drawn at 50% probability.

This is the second picdien complex in which the metal is pentacoordinated; there are some appreciable differences in the ligand between these and the hexacoordinated octahedral picdien complexes, for example the C—N (secondary) bond lengths tend to be shorter in the pentacoordinate complexes and this is especially noticeable in the zinc complex. On the other hand, the bond angles about these N atoms also tend to be slightly larger in the pentacoordinate zinc and copper complexes (Rosales, Toscano, Luna-Canut & Sosa-Torres, 1989) than in the corresponding chromium and cobalt compounds (Bombieri, Forsellini, Del Pra, Tobe, Chatterjee & Cooksey, 1983). Both trends can be understood in terms of the different steric demands on the ligand. This is also reflected in the torsion angles (Table 2). N(2) and N(4) are chiral having *R* and *S* configurations in the enantiomer drawn in Fig. 1. Torsion angles for the pentanuclear chelate rings indicate that they are quite distorted, not fitting either regular envelope or half-chair conformations (Bucourt, 1974).

The anionic $[ZnCl_4]^{2-}$ complex shows a nearly regular tetrahedral structure with a mean Zn—Cl bond distance of 2.2685 Å, not unlike that previously observed in $[Cr(picdien)Cl][ZnCl_4]$. Some short intermolecular interactions are observed between the chloride ions and the nitrogen-bonded protons with H···Cl distances ranging from 2.737 to 2.946 Å.

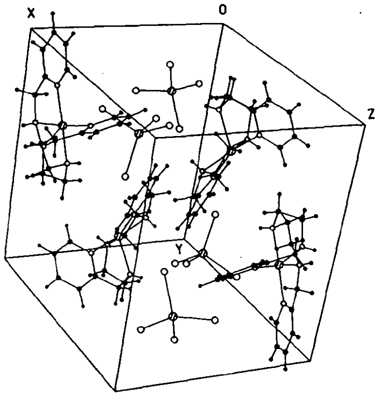

Fig. 2. Crystal packing in [Zn(picdien)][ZnCl$_4$].

Experimental

Crystal data

$C_{16}H_{23}N_5Zn.Cl_4Zn$
M_r = 557.96
Monoclinic
$P2_1/n$
a = 11.656 (4) Å
b = 13.798 (5) Å
c = 13.738 (5) Å
β = 92.45 (3)°
V = 2207 (1) Å^3
Z = 4
D_x = 1.68 Mg m^{-3}

Cu $K\alpha$ radiation
λ = 1.5418 Å
Cell parameters from 25 reflections
θ = 4.8–14.5°
μ = 7.398 mm^{-1}
T = 293 K
Prism
0.36 × 0.34 × 0.32 mm
Colorless

Data collection

Nicolet $R3m$ diffractometer
$2\theta/\theta$ scans
Absorption correction: empirical
T_{min} = 0.004, T_{max} = 0.042
3104 measured reflections
2787 independent reflections
2601 observed reflections [$F>3\sigma(F)$]

R_{int} = 0.079
θ_{max} = 55°
$h = 0 \rightarrow 12$
$k = 0 \rightarrow 14$
$l = -14 \rightarrow 14$
2 standard reflections monitored every 50 reflections intensity variation: <3%

Refinement

Refinement on F
Final R = 0.072
wR = 0.078
S = 1.471
2601 reflections
253 parameters
$w = 1/[\sigma^2(F_o)+0.00419(F_o)^2]$

$(\Delta/\sigma)_{max}$ = 0.402
$\Delta\rho_{max}$ = 0.82 e Å^{-3}
$\Delta\rho_{min}$ = −0.52 e Å^{-3}
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters* (Å^2)

U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Zn(1)	0.2342 (1)	0.2821 (1)	0.0171 (1)	0.076 (1)
Zn(2)	0.5695 (1)	0.7997 (1)	0.2578 (1)	0.077 (1)
Cl(1)	0.3072 (2)	0.1399 (1)	0.0723 (1)	0.095 (1)
Cl(2)	0.0485 (1)	0.2802 (1)	−0.0357 (1)	0.085 (1)
Cl(3)	0.2479 (1)	0.3963 (1)	0.1376 (1)	0.087 (1)
Cl(4)	0.3424 (1)	0.3298 (1)	−0.1086 (1)	0.086 (1)
N(1)	0.7402 (4)	0.8314 (4)	0.3074 (4)	0.078 (2)
N(2)	0.5419 (4)	0.9256 (3)	0.3467 (3)	0.077 (2)
N(3)	0.5424 (5)	0.9006 (4)	0.1424 (4)	0.088 (2)
N(4)	0.4026 (5)	0.7541 (4)	0.2062 (4)	0.087 (2)
N(5)	0.5585 (4)	0.6639 (3)	0.3251 (3)	0.074 (1)
C(1)	0.8370 (5)	0.7890 (4)	0.2779 (5)	0.087 (2)
C(2)	0.9411 (6)	0.8088 (5)	0.3219 (5)	0.097 (2)
C(3)	0.9484 (6)	0.8740 (5)	0.3940 (5)	0.100 (3)
C(4)	0.8523 (5)	0.9176 (5)	0.4232 (5)	0.087 (2)
C(5)	0.7487 (5)	0.8948 (4)	0.3794 (4)	0.078 (2)
C(6)	0.6386 (5)	0.9395 (5)	0.4139 (5)	0.089 (2)
C(7)	0.5141 (6)	1.0070 (4)	0.2814 (4)	0.087 (2)
C(8)	0.5705 (6)	0.9967 (4)	0.1856 (5)	0.091 (2)
C(9)	0.4277 (7)	0.8922 (5)	0.1011 (5)	0.106 (3)
C(10)	0.3830 (7)	0.7927 (5)	0.1068 (5)	0.102 (3)
C(11)	0.3914 (6)	0.6481 (5)	0.2156 (5)	0.089 (2)
C(12)	0.4726 (5)	0.6078 (4)	0.2913 (4)	0.080 (2)
C(13)	0.4644 (7)	0.5140 (5)	0.3220 (5)	0.102 (3)
C(14)	0.5480 (7)	0.4760 (5)	0.3886 (5)	0.110 (3)
C(15)	0.6332 (7)	0.5355 (6)	0.4208 (5)	0.106 (3)
C(16)	0.6374 (6)	0.6289 (5)	0.3910 (4)	0.085 (2)

Table 2. *Bond lengths* (Å), *angles* (°) *and selected torsion angles* (°)

Zn(1)—Cl(1)	2.257 (2)	Zn(1)—Cl(2)	2.253 (2)
Zn(1)—Cl(3)	2.286 (2)	Zn(1)—Cl(4)	2.278 (2)
Zn(2)—N(1)	2.121 (4)	Zn(2)—N(2)	2.155 (5)
Zn(2)—N(3)	2.124 (6)	Zn(2)—N(4)	2.137 (6)
Zn(2)—N(5)	2.096 (4)	N(1)—C(1)	1.348 (8)
N(1)—C(5)	1.321 (8)	N(2)—C(6)	1.439 (7)
N(2)—C(7)	1.464 (8)	N(3)—C(8)	1.483 (8)
N(3)—C(9)	1.435 (10)	N(4)—C(10)	1.473 (9)
N(4)—C(11)	1.475 (9)	N(5)—C(12)	1.334 (7)
N(5)—C(16)	1.352 (8)	C(1)—C(2)	1.360 (9)
C(2)—C(3)	1.337 (10)	C(3)—C(4)	1.348 (10)
C(4)—C(5)	1.363 (8)	C(5)—C(6)	1.518 (9)
C(7)—C(8)	1.503 (9)	C(9)—C(10)	1.471 (10)
C(11)—C(12)	1.483 (9)	C(12)—C(13)	1.366 (9)
C(13)—C(14)	1.409 (11)	C(14)—C(15)	1.349 (11)
C(15)—C(16)	1.354 (10)		
Cl(1)—Zn(1)—Cl(2)	116.2 (1)	Cl(1)—Zn(1)—Cl(3)	110.0 (1)
Cl(2)—Zn(1)—Cl(3)	106.1 (1)	Cl(1)—Zn(1)—Cl(4)	107.0 (1)
Cl(2)—Zn(1)—Cl(4)	108.4 (1)	Cl(3)—Zn(1)—Cl(4)	109.0 (1)
N(1)—Zn(2)—N(2)	79.2 (2)	N(1)—Zn(2)—N(3)	102.2 (2)
N(2)—Zn(2)—N(3)	82.7 (2)	N(1)—Zn(2)—N(4)	174.7 (2)
N(2)—Zn(2)—N(4)	105.6 (2)	N(3)—Zn(2)—N(4)	80.8 (2)
N(1)—Zn(2)—N(5)	96.7 (2)	N(2)—Zn(2)—N(5)	117.2 (2)
N(3)—Zn(2)—N(5)	154.9 (2)	N(4)—Zn(2)—N(5)	79.1 (2)
Zn(2)—N(1)—C(1)	126.8 (4)	Zn(2)—N(1)—C(5)	114.6 (4)
C(1)—N(1)—C(5)	118.4 (5)	Zn(2)—N(2)—C(6)	109.8 (4)
Zn(2)—N(2)—C(7)	107.8 (3)	C(6)—N(2)—C(7)	115.9 (5)
Zn(2)—N(3)—C(8)	105.3 (4)	Zn(2)—N(3)—C(9)	110.4 (4)
C(8)—N(3)—C(9)	114.7 (6)	Zn(2)—N(4)—C(10)	107.7 (4)
Zn(2)—N(4)—C(11)	110.2 (4)	C(10)—N(4)—C(11)	115.4 (5)
Zn(2)—N(5)—C(12)	115.1 (4)	Zn(2)—N(5)—C(16)	124.2 (4)
C(12)—N(5)—C(16)	120.4 (5)	N(1)—C(1)—C(2)	121.4 (6)
C(1)—C(2)—C(3)	119.5 (7)	C(2)—C(3)—C(4)	119.5 (6)
C(3)—C(4)—C(5)	119.8 (6)	N(1)—C(5)—C(4)	121.4 (5)
N(1)—C(5)—C(6)	117.8 (5)	C(4)—C(5)—C(6)	120.8 (5)
N(2)—C(6)—C(5)	113.3 (5)	N(2)—C(7)—C(8)	111.7 (5)
N(3)—C(8)—C(7)	109.7 (5)	N(3)—C(9)—C(10)	112.4 (6)
N(4)—C(10)—C(9)	110.2 (6)	N(4)—C(11)—C(12)	112.2 (5)
N(5)—C(12)—C(11)	118.3 (5)	N(5)—C(12)—C(13)	120.2 (6)
C(11)—C(12)—C(13)	121.4 (6)	C(12)—C(13)—C(14)	119.8 (7)
C(13)—C(14)—C(15)	117.8 (7)	C(14)—C(15)—C(16)	121.0 (7)
N(5)—C(16)—C(15)	120.7 (6)		

N(1)—C(5)—C(6)—N(2)	−15.3 (8)
N(2)—C(7)—C(8)—N(3)	53.1 (7)
N(3)—C(9)—C(10)—N(4)	48.7 (8)
N(4)—C(11)—C(12)—N(5)	−13.9 (8)
C(5)—C(6)—N(2)—C(7)	−98.1 (6)
C(6)—N(2)—C(7)—C(8)	93.6 (6)
C(7)—C(8)—N(3)—C(9)	74.9 (7)

C(8)—N(3)—C(9)—C(10)	−149.8 (6)
C(9)—C(10)—N(4)—C(11)	−163.9 (6)
C(10)—N(4)—C(11)—C(12)	145.7 (6)

The H atoms of the CH_2 and pyridyl groups were allowed to ride on the C atoms to which they are bonded. The H atoms bonded to N atoms were found on a difference Fourier map at an advanced stage of refinement and their coordinates refined.

Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and torsion angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55708 (17 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: CR1007]

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Tetrachlorobis(2-pyridone)-bis-(μ_2-2-pyridone)-dicopper

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Abstract

In this structure two Cu^{II} centres 3.4448 (11) Å apart are bridged asymmetrically by two 2-pyridone ligands and each is further coordinated by three terminal ligands (two chlorides and one 2-pyridone). Each molecule has an approximate, non-crystallographic centre of symmetry. The molecule has two internal hydrogen bonds, each of which involves the oxygen of a terminal pyridone and the amide hydrogen of the adjacent bridging ligand with distances N···O = 2.831 (7), N···O = 2.731 (7) Å. Each pair of molecules is linked by two intermolecular contacts to form infinite chains: N···Cl^i = 3.244 (5), Cl···N^i = 3.269 (5) Å. Symmetry operation i = 1 + *x*, *y*, *z*.

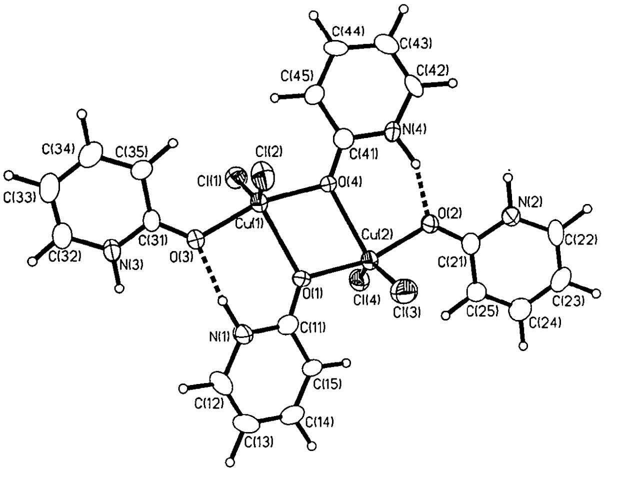

Fig. 1. View of the molecule showing the labelling scheme used. Thermal ellipsoids are drawn at the 50% probability level, excepting those of H which are shown with arbitrary radii. The intramolecular hydrogen bonds are shown as dotted lines.

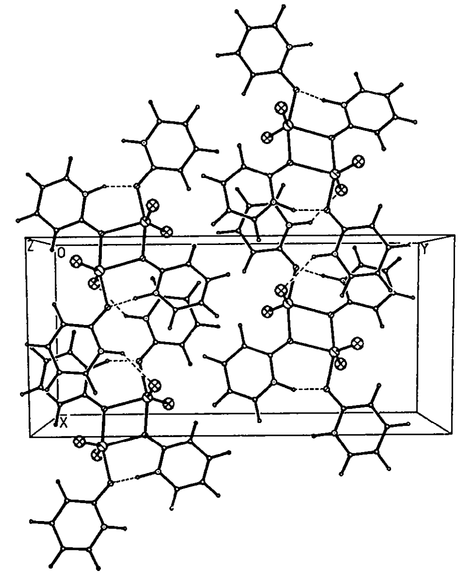

Fig. 2. Packing diagram showing the chains formed *via* intermolecular hydrogen bonding.

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