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Triaqua(5-methyl-1*H*-tetrazolato-κN^1)-zinc(II) perchlorate

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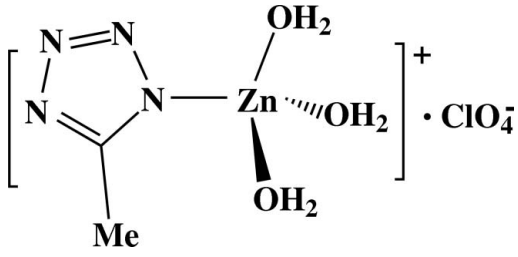
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.009 Å; R factor = 0.049; wR factor = 0.114; data-to-parameter ratio = 12.1.

The title compound, $[Zn(C_2H_3N_4)(H_2O)_3]ClO_4$, consists of one Zn^{II} complex cation and one uncoordinated perchlorate anion. Both anion and cation lie on mirror planes. The Zn^{II} ion displays a distorted tetrahedral geometry and is coordinated by three O atoms and one N atom. Classical O—H···O and O—H···N hydrogen-bond interactions connect cations and anions to form a one-dimensional chain along [010].

Related literature

For related literature, see: Carlucci *et al.* (1999); Demko & Sharpless (2001); Xiong *et al.* (2002).



Experimental

Crystal data

$[Zn(C_2H_3N_4)(H_2O)_3]ClO_4$
M_r = 301.95
Monoclinic, $P2_1/m$
a = 6.1055 (5) Å
b = 7.6413 (6) Å
c = 11.6547 (9) Å
β = 101.220 (2)°
V = 533.35 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.58 mm^{-1}
T = 291 (2) K
0.18 × 0.14 × 0.12 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.66, T_{max} = 0.73
3060 measured reflections
1133 independent reflections
1034 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.114
S = 1.10
1133 reflections
94 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.70 e Å^{-3}
$\Delta\rho_{min}$ = −0.61 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2C···O3^{i}	0.87 (6)	2.33 (6)	3.050 (4)	140 (5)
O1—H1A···N2^{ii}	0.85 (6)	2.61 (6)	3.202 (6)	127 (5)
O1—H1B···O3^{iii}	0.86 (7)	2.29 (7)	2.982 (5)	138 (5)

Symmetry codes: (i) $x, y-1, z$; (ii) $x+1, y, z$; (iii) $x+1, y-1, z$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2000); program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The authors are grateful to the Starter Fund of Southeast University for financial support to buy the CCD X-ray diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2109).

References

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Demko, Z. P. & Sharpless, K. B. (2001). *J. Org. Chem.* **66**, 7945–7950.
Xiong, R.-G., Xue, X., Zhao, H., You, X.-Z., Abrahams, B. F. & Xue, Z. (2002). *Angew. Chem. Int. Ed.* **41**, 3800–3803.

supplementary materials

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Triaqua(5-methyl-1*H*-tetrazolato-κN^1)zinc(II) perchlorate

D.-W. Fu and H. Zhao

Comment

The tetrazole functional group has found a wide range of applications as ligand in coordination chemistry, in medicinal chemistry as a metabolically stable surrogate for a carboxylic acid group, and in material sciences as high density energy materials (Carlucci *et al.*, 1999; Demko & Sharpless, 2001). Recently, we have successfully trapped and structurally characterized many intermediates in which organic part contains one or two cyano groups, affording mono-tetrazolyl or bi-tetrazolyl organic ligands (Xiong *et al.*, 2002). Herein, we report the crystal structure of a simple tetrazole coordination compound, (I), synthesized *in-situ* by hydrothermal method.

The crystal structure shows that the title compound presents a novel structure consisting of two distinct units: the coordination Zn^{II} complex cation and the perchlorate anion, both lying on a mirror plane. For the cation, atoms in special positions are C1/C2/N1/N2/N3/N4/Zn1/O2, while O1 is in general position. The Zn^{II} ion is in a distorted tetrahedral geometry and is coordinated to three O atoms from water molecules and one N atom from the tetrazolate ring (Fig.1). It should be noted that there are classical O—H···O and O—H···N hydrogen bond interactions in the crystal structure (Table 1, Fig. 2). Owning to the intermolecular hydrogen bonding interactions, the cations and the anions are linked into a one-dimensional (one-dimensional) backbone chain along [010] axis (Fig, 3). Finally, adjacent chains are further extended into a three-dimensional (three-dimensional) network structure through weak contacts.

Experimental

The hydrothermal treatment of acetonitrile (8.2 mg, 0.2 mmol), $Zn(ClO_4)_2$ (26.4 mg, 0.1 mmol), and NaN_3 (32.5 mg, 0.5 mmol) in water (2 ml) for 1 day at 1473 K afforded colourless crystals of the title complex.

Refinement

H atoms bonded to O atoms were located in a difference map and refined with free coordinates and U_{iso}(H) = 1.2U_{eq}(carrier O). The methyl H atoms were positioned geometrically and refined using a riding model, with C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C2).

Figures

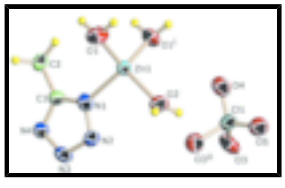

Fig. 1. The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Symmetry codes: (*i*) *x*, −1/2 − *y*, *z*; (*ii*) *x*, 1/2 − *y*, *z*.

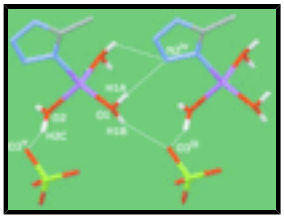

Fig. 2. View of the hydrogen bond interactions in the crystal structure. Symmetry codes: (*iii*) $x+1, y-1, z$; (*iv*) $x+1, y, z$; (*v*) $x, y-1, z$.

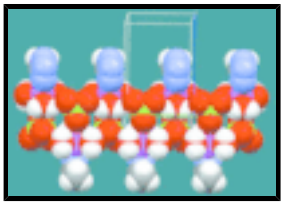

Fig. 3. View of the one-dimensional helix chain along axis [010].

Triaqua(5-methyl-1*H*-tetrazolato-κN^1)zinc(II) perchlorate

Crystal data

$[Zn(C_2H_3N_4)(H_2O)_3]ClO_4$	$F_{000} = 304$
$M_r = 301.95$	$D_x = 1.880$ Mg m^{-3}
Monoclinic, $P2_1/m$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2yb	Cell parameters from 746 reflections
$a = 6.1055$ (5) Å	$\theta = 2.1$–23.6º
$b = 7.6413$ (6) Å	$\mu = 2.58$ mm^{-1}
$c = 11.6547$ (9) Å	$T = 291$ (2) K
$\beta = 101.220$ (2)º	Block, colourless
$V = 533.35$ (7) Å^3	0.18 × 0.14 × 0.12 mm
$Z = 2$	

Data collection

Bruker SMART APEX CCD diffractometer	1133 independent reflections
Radiation source: sealed tube	1034 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.035$
$T = 291(2)$ K	$\theta_{max} = 26.0$º
φ and ω scans	$\theta_{min} = 3.2$º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	$h = -7 \rightarrow 7$
$T_{min} = 0.66$, $T_{max} = 0.73$	$k = -9 \rightarrow 9$
3060 measured reflections	$l = -14 \rightarrow 10$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.049$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.114$	$w = 1/[\sigma^2(F_o^2) + (0.06P)^2 + 0.88P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.10$	$(\Delta/\sigma)_{max} < 0.001$
1133 reflections	$\Delta\rho_{max} = 0.70$ e Å^{-3}
94 parameters	$\Delta\rho_{min} = -0.61$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.4977 (10)	0.2500	0.5068 (6)	0.0331 (13)
C2	0.7244 (10)	0.2500	0.5742 (5)	0.0360 (15)
H2A	0.8278	0.2500	0.5218	0.054*
H2B	0.7477	0.3526	0.6227	0.054*
Cl1	0.2413 (2)	0.7500	0.08687 (14)	0.0362 (4)
N1	0.4385 (9)	0.2500	0.3991 (5)	0.0353 (12)
N2	0.2200 (8)	0.2500	0.3701 (4)	0.0345 (12)
N3	0.1563 (9)	0.2500	0.4728 (5)	0.0404 (14)
N4	0.3248 (9)	0.2500	0.5603 (4)	0.0334 (12)
O1	0.7816 (6)	0.0291 (5)	0.2642 (4)	0.0466 (9)
H1B	0.840 (10)	0.025 (9)	0.203 (6)	0.056*
H1A	0.885 (10)	0.032 (9)	0.325 (5)	0.056*
O2	0.3480 (8)	0.2500	0.1219 (4)	0.0449 (12)
H2C	0.291 (9)	0.152 (9)	0.091 (5)	0.054*
O3	0.1365 (6)	0.8932 (5)	0.1446 (3)	0.0489 (9)
O4	0.4596 (8)	0.7500	0.1194 (4)	0.0454 (12)
O5	0.1834 (8)	0.7500	−0.0279 (5)	0.0467 (12)
Zn1	0.59689 (11)	0.2500	0.25880 (6)	0.0268 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.024 (3)	0.041 (4)	0.034 (3)	0.000	0.005 (2)	0.000
C2	0.035 (3)	0.048 (4)	0.022 (3)	0.000	−0.004 (2)	0.000
Cl1	0.0311 (7)	0.0386 (9)	0.0352 (8)	0.000	−0.0024 (6)	0.000
N1	0.041 (3)	0.039 (3)	0.027 (3)	0.000	0.011 (2)	0.000
N2	0.029 (2)	0.050 (3)	0.022 (2)	0.000	0.000 (2)	0.000
N3	0.034 (3)	0.054 (4)	0.038 (3)	0.000	0.019 (2)	0.000
N4	0.032 (3)	0.045 (3)	0.024 (2)	0.000	0.007 (2)	0.000
O1	0.0413 (19)	0.042 (2)	0.058 (2)	0.0146 (16)	0.0145 (16)	−0.0136 (18)
O2	0.031 (2)	0.068 (4)	0.034 (3)	0.000	0.002 (2)	0.000
O3	0.053 (2)	0.049 (2)	0.051 (2)	−0.0228 (17)	0.0246 (17)	−0.0069 (17)
O4	0.052 (3)	0.042 (3)	0.047 (3)	0.000	0.022 (2)	0.000
O5	0.043 (3)	0.052 (3)	0.045 (3)	0.000	0.007 (2)	0.000
Zn1	0.0265 (4)	0.0311 (4)	0.0236 (4)	0.000	0.0071 (2)	0.000

Geometric parameters (Å, °)

C1—N1	1.237 (8)	N1—Zn1	2.055 (5)
C1—N4	1.326 (8)	N2—N3	1.330 (8)
C1—C2	1.453 (8)	N3—N4	1.300 (8)
C2—H2A	0.9600	O1—Zn1	2.024 (3)
C2—H2B	0.9600	O1—H1B	0.86 (7)
Cl1—O4	1.313 (5)	O1—H1A	0.85 (6)
Cl1—O5	1.315 (5)	O2—Zn1	1.977 (5)
Cl1—O3	1.493 (4)	O2—H2C	0.87 (6)
Cl1—O3^{i}	1.493 (4)	Zn1—O1^{ii}	2.024 (3)
N1—N2	1.311 (7)		
N1—C1—N4	112.0 (6)	N2—N1—Zn1	114.1 (4)
N1—C1—C2	127.5 (6)	N1—N2—N3	103.2 (5)
N4—C1—C2	120.5 (6)	N4—N3—N2	112.4 (5)
C1—C2—H2A	109.3	N3—N4—C1	102.3 (5)
C1—C2—H2B	109.5	Zn1—O1—H1B	109 (5)
H2A—C2—H2B	109.5	Zn1—O1—H1A	109 (5)
O4—Cl1—O5	110.5 (3)	H1B—O1—H1A	109 (6)
O4—Cl1—O3	111.7 (2)	Zn1—O2—H2C	121 (4)
O5—Cl1—O3	113.9 (2)	O2—Zn1—O1^{ii}	111.18 (13)
O4—Cl1—O3^{i}	111.7 (2)	O2—Zn1—O1	111.18 (13)
O5—Cl1—O3^{i}	113.9 (2)	O1^{ii}—Zn1—O1	113.0 (2)
O3—Cl1—O3^{i}	94.3 (3)	O2—Zn1—N1	103.6 (2)
C1—N1—N2	110.1 (5)	O1^{ii}—Zn1—N1	108.70 (14)
C1—N1—Zn1	135.9 (5)	O1—Zn1—N1	108.70 (14)

Symmetry codes: (i) *x*, −*y*+3/2, *z*; (ii) *x*, −*y*+1/2, *z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2C···O3^{iii}	0.87 (6)	2.33 (6)	3.050 (4)	140 (5)
O1—H1A···N2^{iv}	0.85 (6)	2.61 (6)	3.202 (6)	127 (5)
O1—H1B···O3^{v}	0.86 (7)	2.29 (7)	2.982 (5)	138 (5)

Symmetry codes: (iii) *x*, *y*−1, *z*; (iv) *x*+1, *y*, *z*; (v) *x*+1, *y*−1, *z*.

Fig. 1

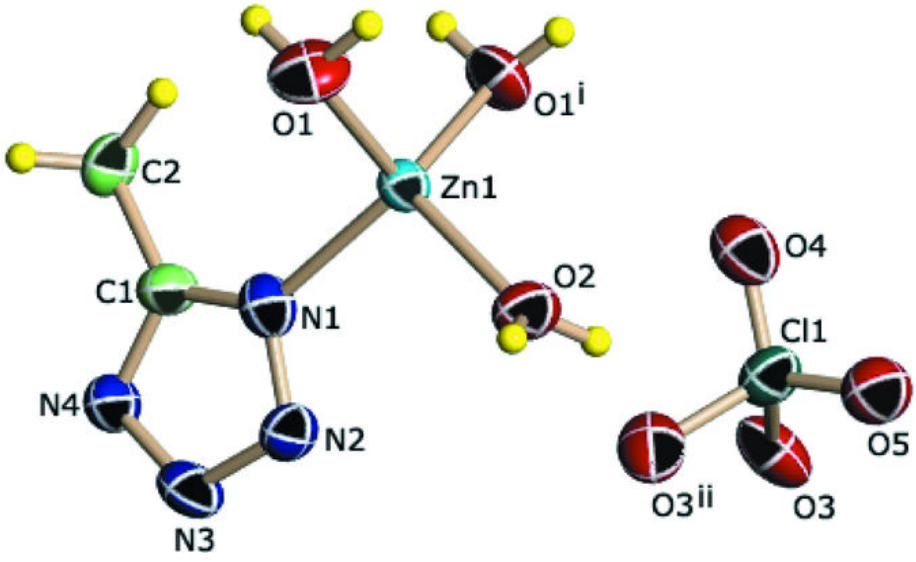

Fig. 2

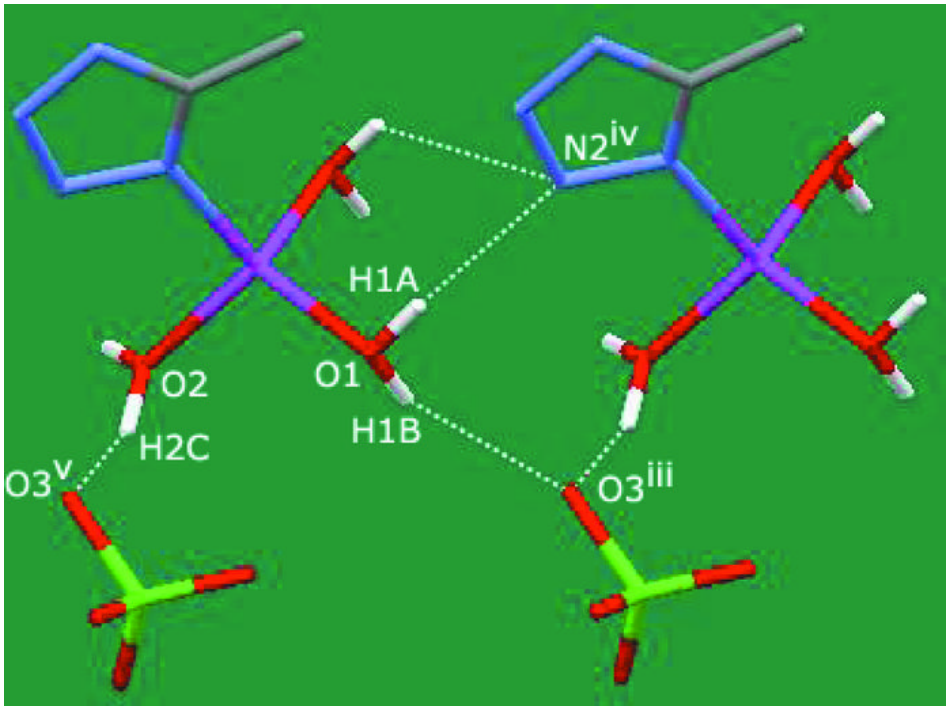

Fig. 3