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Hexaaquazinc(II) bis(perchlorate) bis(2,5-dimethylpyrazine 1,4-dioxide)

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The title molecular complex, $[Zn(H_2O)_6](ClO_4)_2\cdot 2C_6H_8N_2O_2$, consists of neutral 2,5-dimethylpyrazine 1,4-dioxide molecules, a hexaaquazinc(II) cation and perchlorate anions, linked through Coulombic attraction and hydrogen bonding. Half the neutral molecules lie in general positions, and the other half are on inversion centers.

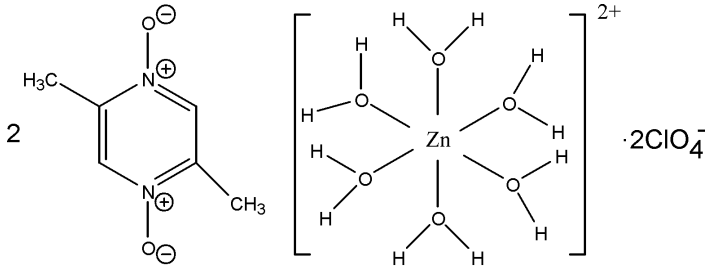
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.007 Å
R factor = 0.054
wR factor = 0.141
Data-to-parameter ratio = 12.4

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

Comment

In the crystal structure of the title complex, (I), the zinc(II) ion is coordinated by six water molecules and has distorted octahedral geometry (Fig. 1). The coordinated water molecules are involved in extensive hydrogen-bonding interactions with both the perchlorate O atoms and the 2,5-dimethylpyrazine 1,4-dioxide molecules. The asymmetric unit consists of one cation, two anions, a neutral molecule in a general position, and halves of two separate centrosymmetric neutral molecules. In addition, there is Coulombic attraction between the hexaaquazinc(II) cation and the perchlorate anions. The hydrogen bonds which connect the three components in the crystal structure are shown in Fig. 2. In the crystal structure, the hexaaquazinc(II) cations and 2,5-dimethylpyrazine 1,4-dioxide molecules are each stacked in an orderly manner along the b axis, forming infinite columns. Each hexaaquazinc(II) column is surrounded by four 2,5-dimethylpyrazine 1,4-dioxide columns and perchlorate anions are inserted into the columns of 2,5-dimethylpyrazine 1,4-dioxide molecules.



(I)

Experimental

To an aqueous solution (8 ml) containing $[Zn(H_2O)_6](ClO_4)_2$ (0.0760 g, 0.204 mmol), 2,5-dimethylpyrazine 1,4-dioxide (0.0860 g, 0.614 mmol) was added and the resulting solution stirred for a few minutes. Colorless single crystals were obtained after the solution was allowed to stand at room temperature for three weeks.

Crystal data

$[Zn(H_2O)_6](ClO_4)_2\cdot 2C_6H_8N_2O_2$
$M_r = 652.65$
Orthorhombic, *Pbcn*
$a = 19.700$ (4) Å
$b = 13.097$ (3) Å
$c = 20.021$ (4) Å
$V = 5166$ (2) Å^3
$Z = 8$
$D_x = 1.678$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3876 reflections
$\theta = 2.9$–24.2°
$\mu = 1.24$ mm^{-1}
$T = 298$ (2) K
Rectangular block, colorless
0.50 × 0.15 × 0.11 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.575$, $T_{max} = 0.875$
26350 measured reflections
4805 independent reflections
3802 reflections with $I > 2\sigma(I)$
$R_{int} = 0.061$
$\theta_{max} = 25.5^\circ$
$h = -23 \rightarrow 23$
$k = -15 \rightarrow 15$
$l = -24 \rightarrow 22$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.142$
$S = 1.06$
4805 reflections
386 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0678P)^2 + 6.6643P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.88$ e Å^{-3}
$\Delta\rho_{min} = -0.82$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H1O3···O12^{i}	0.85 (3)	1.954 (17)	2.789 (5)	168 (5)
O4—H1O4···O8^{i}	0.85 (4)	1.96 (2)	2.772 (4)	160 (5)
O5—H2O5···O8^{ii}	0.85 (5)	1.93 (5)	2.754 (5)	165 (5)
O1—H2O1···O7	0.85 (5)	1.89 (5)	2.688 (4)	157 (5)
O6—H2O6···O13	0.84 (3)	2.08 (2)	2.895 (5)	161 (5)
O2—H2O2···O15	0.86 (4)	1.94 (4)	2.785 (5)	171 (6)
O2—H2O2···Cl3	0.86 (4)	2.82 (4)	3.548 (3)	144 (5)
O5—H1O5···O16^{iii}	0.84 (3)	2.04 (2)	2.839 (8)	157 (5)
O4—H2O4···O10^{i}	0.85 (3)	1.901 (17)	2.721 (4)	163 (4)
O3—H2O3···O10^{ii}	0.85 (3)	1.90 (3)	2.744 (5)	173 (6)
O1—H1O1···O9	0.85 (3)	1.93 (4)	2.774 (4)	177 (5)
O6—H1O6···O7^{iv}	0.849 (11)	1.841 (12)	2.688 (4)	175 (5)
O2—H1O2···O9^{iv}	0.85 (3)	1.846 (15)	2.688 (5)	169 (5)

Symmetry codes: (i) $\frac{1}{2}-x, \frac{3}{2}-y, \frac{1}{2}+z$; (ii) $x, 1-y, \frac{1}{2}+z$; (iii) $x-\frac{1}{2}, \frac{3}{2}-y, 1-z$; (iv) $\frac{1}{2}-x, \frac{1}{2}+y, z$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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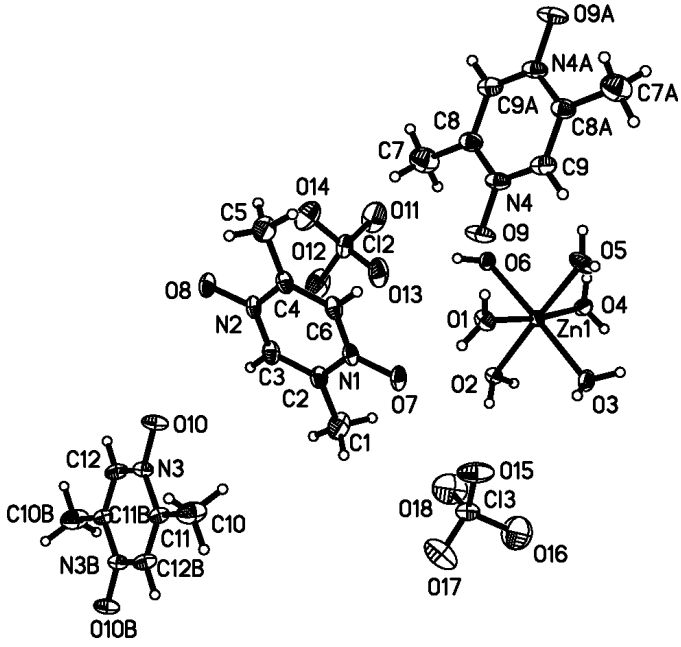

Figure 1
The title complex, with 30% probability displacement ellipsoids. H atoms are shown as small spheres of arbitary radii. [Symmetry codes: (*A*) $-x, -y+1, -z+1$; (*B*) $-x+1, -y+1, -z$.]

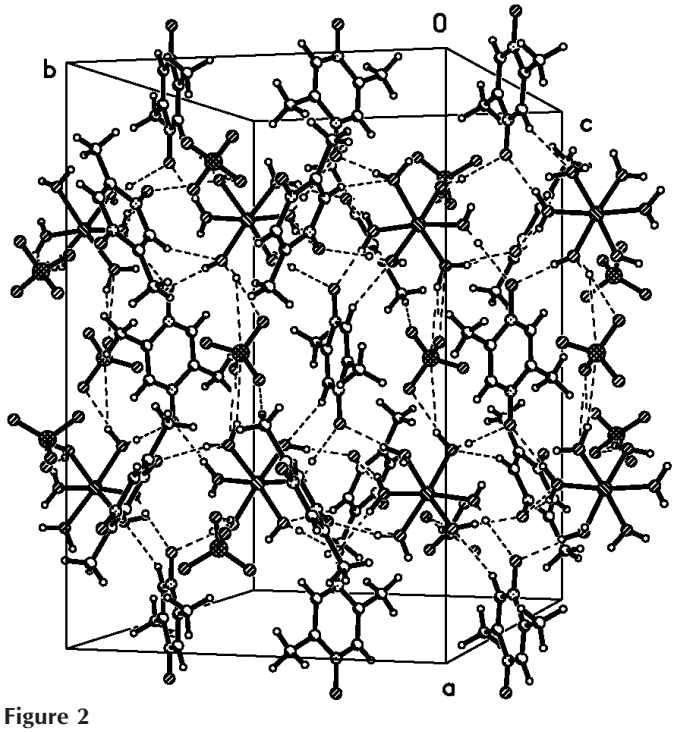

Figure 2
The packing of (I), with hydrogen bonds shown as dashed lines.

References

Bruker (1997). *SMART* (Version 5.6) and *SAINT* (Version 5.A06). Bruker AXS Inc., Madison, Wisconsin, USA.

Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.

Sheldrick, G. M. (2001). *SHELXTL*. Version 6.12. Bruker AXS Inc., Masison, Wisconsin, USA.