Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Ethane-1,2-diaminium hexaaquazinc(II) sulfate

Apinpus Rujiwatra[a]* and Jumras Limtrakul[b]

[a]Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai 50200, Thailand, and [b]Department of Chemistry, Faculty of Science, Kasetsart University, Bangkok 10900, Thailand

Correspondence e-mail:
apinpus@chiangmai.ac.th

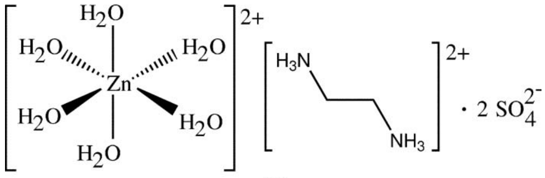
Received 17 May 2005
Accepted 21 June 2005
Online 24 June 2005

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.024
wR factor = 0.064
Data-to-parameter ratio = 13.9

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

The crystal structure of the title compound, $(C_2H_{10}N_2)$-$[Zn(H_2O)_6]$>$(SO_4)_2$, comprises Zn^{II} complex cations, sulfate anions and diprotonated ethane-1,2-diamine (DAE). The Zn^{II} atom is located on an inversion centre and is coordinated by six water molecules in an octahedral geometry. The DAE dication is located on another inversion centre. Hydrogen bonding occurs between anions and cations but not between DAE and Zn^{II} complex cations.



(I)

Experimental

The reaction mixture was prepared by dissolving $ZnSO_4{\cdot}7H_2O$ (RDH 98%) in ethanol (Merck 95%), into which ethylenediamine, en (Carlo Erba 98%), was added while stirring vigorously. A white precipitate with a compositional molar ratio of $ZnSO_4{\cdot}7H_2O$:en:C_2H_5OH 1:0.1:100 was formed. The mixture was refluxed at 353 K for 6 h before allowing it to cool to room temperature. The white precipitate did not dissolve and was separated from the clear solution, into which an equivalent volume of deionized water was added. On storing at room temperature, single crystals of (I) were obtained from the solution after 24 h. Due to the acidic properties of the starting reagent, $ZnSO_4{\cdot}7H_2O$ and ethanol, protonation of en was assumed and confirmed from Fourier-transform IT spectroscopy (FT–IR) using a Nicolet 510 F T–IR spectrophotometer over the range 4000–400 cm^{-1}. Samples were prepared as KBr pellets. The FT–IR spectrum showed a deformation band characteristic of NH_3^+ at 2100 cm^{-1} and a shoulder centred at 2800 cm^{-1} corresponding to NH stretching shifted to a lower wavenumber due to protonation of the amino group.

Crystal data

$(C_2H_{10}N_2)[Zn(H_2O)_6](SO_4)_2$
M_r = 427.71
Monoclinic, $P2_1/n$
a = 8.1827 (6) Å
b = 7.0914 (5) Å
c = 13.1674 (9) Å
β = 101.154 (1)°
V = 749.63 (9) Å^3
Z = 2
D_x = 1.895 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1676 reflections
θ = 1.6–28.2°
μ = 1.99 mm^{-1}
T = 293 (2) K
Needle, colourless
0.17 × 0.05 × 0.03 mm

Data collection

Nonius KappaCCD diffractometer
φ and ω scans
Absorption correction: none
3753 measured reflections
1352 independent reflections
1308 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 25.2°
$h = -9 \rightarrow 9$
$k = -8 \rightarrow 5$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.024$
$wR(F^2) = 0.064$
$S = 1.14$
1352 reflections
97 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0267P)^2 + 0.7365P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.55$ e Å^{-3}
$\Delta\rho_{\min} = -0.42$ e Å^{-3}

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H3···O5^{i}	0.93	1.82	2.7335 (19)	167
O1—H4···O4^{ii}	0.90	1.84	2.7466 (19)	178
O2—H5···O7^{iii}	0.87	1.98	2.8052 (19)	159
O2—H6···O6	0.90	1.80	2.701 (2)	173
O3—H7···O7^{iii}	0.82	2.14	2.8312 (19)	143
O3—H8···O5^{iv}	0.87	1.87	2.7322 (19)	167
N1—H1*A*···O6^{i}	0.87	2.04	2.856 (2)	156
N1—H1*A*···O5^{i}	0.87	2.50	3.214 (2)	140
N1—H1*B*···O7^{v}	0.91	1.91	2.820 (2)	173
N1—H1*C*···O4	0.80	2.03	2.826 (2)	168

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

H atoms on the N and O atoms were located in a difference Fourier map and were refined as riding in their as-found relative positions to carrier atoms. Methylene H atoms were placed in calculated positions, with C—H = 0.97 Å, and included in the final cycles of refinement in the riding model, with $U_{\rm iso}(\rm H) = 1.5U_{\rm eq}(\rm C)$.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

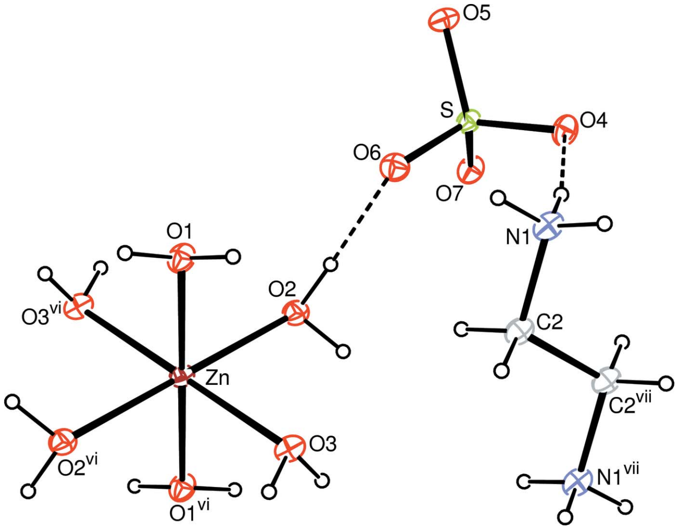


Figure 1
The molecular structure of (I) with 30% probability displacement ellipsoids (arbitrary spheres for H atoms). Dashed lines indicate hydrogen bonds. [Symmetry codes: (vi) $1-x, -y, 1-z$; (vii) $-x, 1-y, 1-z$.]

The authors thank the Thailand Research Fund for research funding.

References

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Nonius (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, Macromolecular Crystallography, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307-326. New York: Academic Press.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.