

Disodium zinc bis(sulfate) tetrahydrate (zinc astrakanite) revisited

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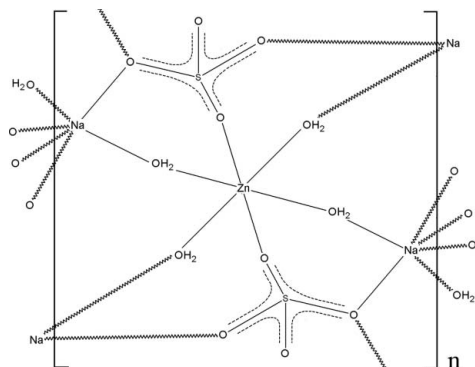
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Key indicators: single-crystal X-ray study; $T = 170$ K; mean $\sigma(\text{S}-\text{O}) = 0.001$ Å; R factor = 0.018; wR factor = 0.055; data-to-parameter ratio = 11.2.

We present a new low-temperature refinement of disodium zinc bis(sulfate) tetrahydrate [systematic name: poly[tetra- μ -aqua-di- μ -sulfato-zinc(II)disodium(I)]], $[\text{Na}_2\text{Zn}(\text{SO}_4)_2(\text{H}_2\text{O})_4]_n$ or Zn astrakanite, which is an upgrade of previously reported data [Bukin & Nozik (1974). *Zh. Strukt. Khim.* **15**, 712–716]. The compound is part of an isostructural family containing the Mg (the original astrakanite mineral), Co and Ni species. The very regular $\text{ZnO}(\text{aqua})_4\text{O}(\text{sulfate})_2$ octahedra lie on centres of symmetry, while the rather distorted $\text{NaO}(\text{aqua})_2\text{O}(\text{sulfate})_4$ octahedra appear at general positions, linked into a three-dimensional network by the bridging water molecules and the fully coordinated sulfate groups.

Related literature

For related literature, see: Rumanova (1958); Giglio (1958); Bukin & Nozik (1974, 1975); Díaz de Vivar *et al.* (2006).



Experimental

Crystal data

$[\text{Na}_2\text{Zn}(\text{SO}_4)_2(\text{H}_2\text{O})_4]$
 $M_r = 375.53$
Monoclinic, $P2_1/c$
 $a = 5.5075$ (2) Å
 $b = 8.2127$ (3) Å
 $c = 11.0559$ (4) Å
 $\beta = 99.958$ (10)°

$V = 492.54$ (3) Å³
 $Z = 2$
Mo $K\alpha$ radiation
 $\mu = 3.07$ mm⁻¹
 $T = 170$ (2) K
 $0.30 \times 0.20 \times 0.10$ mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\text{min}} = 0.452$, $T_{\text{max}} = 0.728$

3533 measured reflections
1080 independent reflections
1062 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.012$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.017$
 $wR(F^2) = 0.054$
 $S = 1.00$
1080 reflections
96 parameters
6 restraints

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.29$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.53$ e Å⁻³

Table 1

Selected bond lengths (Å).

Zn1—O1W	2.0636 (11)	Na1—O1	2.4016 (12)
Zn1—O3	2.0952 (11)	Na1—O1W	2.4017 (12)
Zn1—O2W	2.1285 (11)	Na1—O2 ⁱⁱⁱ	2.4224 (13)
Na1—O2 ⁱ	2.3603 (12)	Na1—O2W ^{iv}	2.5694 (13)
Na1—O4 ⁱⁱ	2.3786 (12)		

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H1WA \cdots O1 ⁱⁱⁱ	0.800 (17)	1.916 (17)	2.6977 (17)	165 (3)
O1W—H1WB \cdots O4 ^v	0.832 (16)	1.901 (16)	2.7288 (17)	173 (2)
O2W—H2WA \cdots O1 ⁱⁱ	0.826 (16)	2.051 (18)	2.8468 (16)	162 (2)
O2W—H2WB \cdots O4 ^{vi}	0.805 (16)	2.15 (2)	2.8779 (16)	151 (3)

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

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL and PLATON (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FI2061).

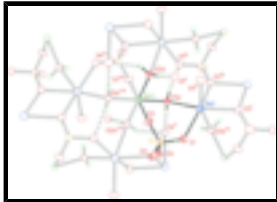
References

- Allen, F. H. (2002). *Acta Cryst.* **B58**, 380–388.
- Bruker (2001). *SMART* and *SAINT* for Windows NT. Bruker AXS Inc., Madison, Wisconsin, USA.
- Bukin, V. I. & Nozik, Yu. Z. (1974). *Zh. Strukt. Khim.* **15**, 712–716.
- Bukin, V. I. & Nozik, Yu. Z. (1975). *Kristallografiya*, **20**, 293–296.
- Díaz de Vivar, M. E., Baggio, S., Garland, M. T. & Baggio, R. (2006). *Acta Cryst.* **E62**, i196–i198.
- Giglio, M. (1958). *Naturwissenschaften*, **45**, 82–83.
- Rumanova, I. M. (1958). *Dokl. Akad. Nauk SSSR*, **118**, 84–87.
- Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

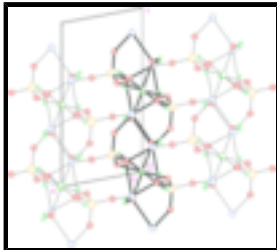
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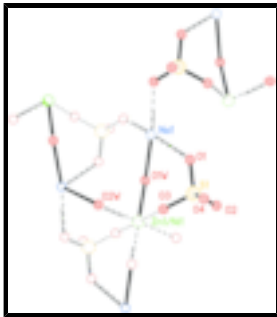
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