Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Na_2ZnGe

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Key indicators

Single-crystal X-ray study
T = 167 K
Mean σ(Ge–Zn) = 0.003 Å
R factor = 0.016
wR factor = 0.033
Data-to-parameter ratio = 33.7

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

Received 19 January 2007
Accepted 24 January 2007

The structure of disodium zinc germanide, Na_2ZnGe, has been determined from single-crystal data and is reported for the first time. The compound crystallizes in the Na_2CuAs structure type. The structure is built of Na^+ ions (8*g* position) and infinite zigzag chains of $(ZnGe)^{2-}$ parallel to the *c* axis (Zn and Ge atoms are in 4*b* and 4*c* positions, respectively).

Comment

The title compound, disodium zinc germanide, Na_2ZnGe, crystallizes in the orthorhombic Na_2CuAs structure type (Eisenmann *et al.*, 1976), as shown in Fig. 1. Na, Zn and Ge atoms are located at special positions 8*g* (0.1748 (1), 0.1406 (1), $\frac{1}{4}$), 4*b* ($\frac{1}{2}$, 0, 0) and 4*c* ($\frac{1}{2}$, 0.2686 (1), $\frac{1}{4}$), respectively. The framework is built of a sodium three-dimensional network forming large channels parallel to the *c* axis which are occupied by infinite zigzag chains of $(ZnGe)^{2-}$. Such chains are isosteric to the ones observed in HgO (Aurivillius, 1956) and have been observed in several isostructural compounds, *viz*. Na_2CuP (Savelsberg & Schäfer, 1977), Na_2AgSb (Schuster *et al.*, 1979), Na_2AuAs, Na_2AuSb and K_2AuSb (Mues & Schuster, 1980), K_2CuP (Eisenmann & Somer, 1985), K_2CuAs and K_2CuSb (Eisenmann *et al.*, 1976), K_2AgP (Asbrand *et al.*, 1997) and K_2AuP (Eisenmann *et al.*, 1991). The compounds K_2AgX with X = As, Sb and Bi (space group $C222_1$; Savelsberg & Schäfer, 1977) and K_2CdX with X = Sn and Pd (space group *Ama2*; Matthes & Schuster, 1979) also contain similar infinite chains, while the two compounds Na_2CdSn (hexagonal, space group $P6_3mmc$) and Na_2CdPb (cubic, $F\bar{4}3m$) exhibit totally different structures that are related to Na_3As and Li_3Bi, respectively (Matthes & Schuster, 1980).

The infinite zigzag chains $(ZnGe)^{2-}$ are built of an alternating arrangement of zinc and germanium atoms and have a twofold screw axis of symmetry, where zinc atoms (formally d^{10}) form linear chains and are linearly coordinated by germanium anions with Zn—Ge bonds of 2.4212 (3) Å and Zn–Ge–Zn angles of 69.211 (1)°. The Zn—Zn distances in the chains of 2.7501 (4) Å are comparable to the ones observed in elemental zinc, *i.e.* 2.67 Å. Both Zn and Ge atoms are eightfold coordinated by sodium cations with 3.4037 (6) Å < Zn—Na < 3.4518 (7) Å and 3.1367 (7) Å < Ge—Na < 3.2556 (7) Å.

Experimental

While investigating the zinc/germanium/nitrogen system, the compound Na_2ZnGe was obtained from the reaction of NaN_3, Zn and Ge with an excess of Na as a flux. Due to the air-sensitivity of the reagents, all manipulations were carried out in an argon-filled glovebox. The starting materials of NaN_3 (0.0852 g, 1.2 mmol), Zn (0.0392 g, 0.6 mmol), Ge (0.0436 g, 0.6 mmol) and Na (0.0552 g,

2.4 mmol) were placed into an Nb tube. The atomic ratio of Na:Zn:Ge:N_2 was 6:1:1:3. The niobium container was sealed under argon in a Centorr Associates arc furnace and then itself sealed under vacuum in a fused silica tube in order to protect it from subsequent oxidation during heating. The silica tube was then placed into a muffle furnace, heated to 1073 K over 15 h and held at this temperature for 1 h. Then the furnace was allowed to cool to room temperature over 100 h. Following the heating step, the niobium tube was opened and unreacted sodium was removed by evaporation from the products by heating the niobium tube to 623 K under a pressure of $\sim 10^{-6}$ bar for 8 h. The remaining product appeared as a bunch of up to 1 mm long thick silvery metallic needles which decomposes within seconds when exposed to air. Some of the needles were ground and analysed by powder X-ray diffraction using a Scintag 2000 θ–θ diffractometer with Cu $K\alpha$ radiation. The powder pattern revealed a well crystallized single phase that could not have been identified using the current crystallographic databases, but matched the calculated pattern from the single-crystal data using *PowderCell 2.2* (Kraus & Nolze, 1996)). The Zn:Ge of 1:1 has been confirmed by microprobe analysis (Jeol JXA-8900R).

Crystal data

Na_2ZnGe	$Z = 4$
$M_r = 183.94$	$D_x = 3.257$ Mg m^{-3}
Orthorhombic, *Cmcm*	Mo $K\alpha$ radiation
$a = 9.1922$ (12) Å	$\mu = 14.37$ mm^{-1}
$b = 7.4198$ (9) Å	$T = 167$ (1) K
$c = 5.5002$ (7) Å	Block cut from a needle, silver
$V = 375.14$ (8) Å^3	0.12 × 0.12 × 0.08 mm

Data collection

Bruker X8 APEX-II 4K CCD area-detector diffractometer	2315 measured reflections 506 independent reflections
φ and ω scans	459 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)	$R_{int} = 0.025$ $\theta_{max} = 36.3°$
$T_{min} = 0.201$, $T_{max} = 0.318$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0139P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.016$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.033$	$\Delta\rho_{max} = 0.45$ e Å^{-3}
$S = 1.12$	$\Delta\rho_{min} = -1.12$ e Å^{-3}
506 reflections	
15 parameters	

The deepest residual electron density hole is located 1.75 Å from atom Na3.

Data collection: *APEX2* (Brucker, 2003); cell refinement: *APEX2*; data reduction: *SAINT-Plus* (Brucker, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

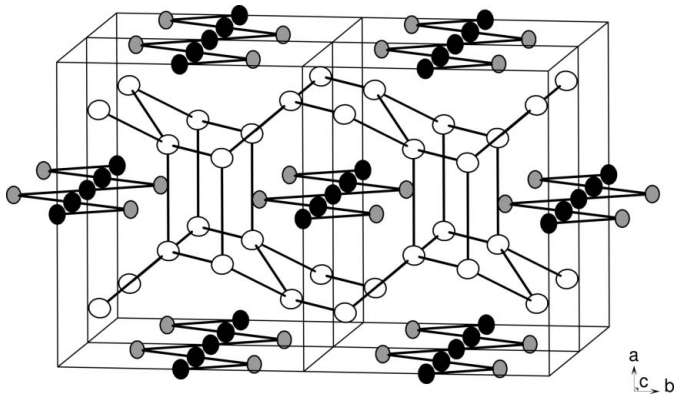

Figure 1
The structure of Na_2ZnGe. Black circles are Zn atoms, gray circles are Ge atoms and open circles are Na atoms. Displacement ellipsoids are drawn at the 90% probability level.

This work was supported by NSF grant number DMR-0602526. We thank Dr. Emil Lobkovsky (single-crystal diffraction) and John Hunt (SEM microprobe) for the use of their facilities. The microprobe is supported by the Cornell Center for Materials Research Shared Experimental Facilities, funded through the National Science Foundation Materials Research Science and Engineering Center Program DMR-0520404.

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