

## The alluaudite-like arsenate NaCaMg<sub>3</sub>(AsO<sub>4</sub>)<sub>3</sub>

Anissa Haj Abdallah\* and Amor Haddad

Laboratoire de Matériaux et Cristallographie, Institut Supérieur des Sciences Appliquées et Technologie de Mahdia, Avenue El Mourouj, Sidi Messoud 5111 Hiboun, Mahdia, Tunisia

Correspondence e-mail: haj\_anissa@yahoo.fr

Received 30 January 2008; accepted 14 May 2008

Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{As}-\text{O}) = 0.003$  Å; disorder in solvent or counterion;  $R$  factor = 0.023;  $wR$  factor = 0.061; data-to-parameter ratio = 11.5.

The title compound, sodium calcium trimagnesium tris(arsenate), an alluaudite-like arsenate, was prepared by solid-state reaction at high temperature. The structure is built up from edge-sharing MgO<sub>6</sub> octahedra in chains associated with the AsO<sub>4</sub> arsenate groups. The three-dimensional network leads to two different tunnels occupied statistically by Na<sup>+</sup> and Ca<sup>2+</sup>. One As and one Mg atom lie on twofold rotation axes; one Na and one Ca are disordered over two sites with occupancies of 0.7 and 0.3 and these sites lie on a twofold rotation axis and an inversion centre, respectively.

### Related literature

For the alluaudite structure type, see: Moore (1971); Yakubovitch *et al.* (1977); Cu<sub>1.35</sub>Fe(PO<sub>4</sub>)<sub>3</sub> (Warner *et al.*, 1993); NaFe<sub>3.67</sub>(PO<sub>4</sub>)<sub>3</sub> (Korzanski *et al.*, 1998). For related alluaudite-like arsenates, see: NaCo<sub>3</sub>(AsO<sub>4</sub>)(HAsO<sub>4</sub>)<sub>2</sub> (Kwang-Hwa & Pei-Fen, 1994); NaCaCdMg<sub>2</sub>(AsO<sub>4</sub>)<sub>3</sub> (Khorari *et al.*, 1997); Ag<sub>1.49</sub>Mn<sub>1.49</sub>Mn<sub>2</sub>(AsO<sub>4</sub>)<sub>3</sub> (Ayed *et al.*, 2002); Na<sub>1.72</sub>Mn<sub>3.28</sub>(AsO<sub>4</sub>)<sub>3</sub> (Brahim *et al.* 2003). For related literature, see: Leroux *et al.* (1995).

### Experimental

#### Crystal data

NaCaMg<sub>3</sub>(AsO<sub>4</sub>)<sub>3</sub> $M_r = 552.74$ 

Monoclinic,  $C2/c$   
 $a = 11.880$  (1) Å  
 $b = 12.817$  (1) Å  
 $c = 6.741$  (2) Å  
 $\beta = 112.45$  (1)°  
 $V = 948.7$  (3) Å<sup>3</sup>

$Z = 4$   
Mo  $K\alpha$  radiation  
 $\mu = 11.36$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 $0.6 \times 0.2 \times 0.15$  mm

#### Data collection

Enraf–Nonius CAD-4 diffractometer  
Absorption correction:  $\psi$  scan (North *et al.*, 1968)  
 $T_{\min} = 0.110$ ,  $T_{\max} = 0.180$   
1358 measured reflections

1154 independent reflections  
1133 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.021$   
2 standard reflections  
frequency: 120 min  
intensity decay: 0.4%

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.022$   
 $wR(F^2) = 0.060$   
 $S = 1.29$   
1154 reflections

100 parameters  
 $\Delta\rho_{\max} = 0.99$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -1.00$  e Å<sup>-3</sup>

Data collection: *CAD-4 EXPRESS* (Duisenberg, 1992; Macíček & Yordanov, 1992); cell refinement: *CAD-4 EXPRESS*; data reduction: *MolEN* (Fair, 1990); program(s) used to solve structure: *SHELXS86* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BR2069).

### References

- Ayed, B., Krifa, M. & Haddad, A. (2002). *Acta Cryst.* **C58**, i98–i100.  
Brahim, A. & Amor, H. (2003). *Acta Cryst.* **E59**, i77–i79.  
Brandenburg, K. (1998). *DIAMOND*. University of Bonn, Germany.  
Duisenberg, A. J. M. (1992). *J. Appl. Cryst.* **25**, 92–96.  
Fair, C. K. (1990). *MolEN*. Enraf–Nonius, Delft, The Netherlands.  
Khorari, S., Rulmont, A., Tarte, P., Miehé, G., Antenucci, D. & Gilbert, B. (1997). *J. Solid State Chem.* **131**, 298–304.  
Korzanski, M. B., Schimek, G. L., Kolis, J. W. & Long, G. J. (1998). *J. Solid State Chem.* **139**, 152–160.  
Kwang-Hwa, L. & Pei-Fen, S. (1994). *Inorg. Chem.* **33**, 3028–3031.  
Leroux, F., Mar, A., Payen, C., Guyomard, D., Verbaere, A. & Piffard, Y. (1995). *J. Solid State Chem.* **115**, 240–246.  
Macíček, J. & Yordanov, A. (1992). *J. Appl. Cryst.* **25**, 73–80.  
Moore, P. B. (1971). *Am. Mineral.* **56**, 1955–1975.  
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* **A24**, 351–359.  
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.  
Warner, T., Milius, W. & Maier, J. (1993). *J. Solid State Chem.* **106**, 301–309.  
Yakubovitch, O. V., Simonov, M. A., Egorov-Tismenko, Y. K. & Belov, N. V. (1977). *Dokl. Akad. Nauk SSSR*, **236**, 1123–1130.

















