

The iron phosphate $\text{NaBaFe}_2(\text{PO}_4)_3$

Mourad Hidouri,* Hasna Jerbi and Mongi Ben Amara

Faculté des Sciences de Monastir, 5019 Monastir, Tunisia

Correspondence e-mail: mourad_hidouri@yahoo.fr

Received 27 May 2008; accepted 22 July 2008

Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{Fe}-\text{O}) = 0.005$ Å; disorder in main residue; R factor = 0.025; wR factor = 0.060; data-to-parameter ratio = 9.4.

A new iron phosphate, sodium barium diiron tris(phosphate), $\text{NaBaFe}_2(\text{PO}_4)_3$, has been synthesized by the flux method and shown to exhibit the well known langbeinite type structure. The Na, Ba and Fe atoms all lie on threefold axes, while the P and O atoms occupy general positions, one of the O atoms being disordered over two positions, with site occupancy factors of *ca* 0.7 and 0.3. The $[\text{Fe}_2(\text{PO}_4)_3]_\infty$ framework consists of FeO_6 octahedra sharing all their corners with the PO_4 tetrahedra. The Na^+ and Ba^{2+} cations are almost equally distributed over two distinct cavities, in which they occupy slightly different positions.

Related literature

For related literature, see: Baur (1974); Moffat (1978); Padhi *et al.* (1997); Shannon (1976). For the structure of langbeinite, see Zemmann & Zemmann (1957); Battle *et al.* (1986, 1988).

Experimental

Crystal data

$\text{NaBaFe}_2(\text{PO}_4)_3$
 $M_r = 556.94$
 Cubic, $P2_13$
 $a = 9.796$ (1) Å
 $V = 940.1$ (3) Å³

$Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 7.82$ mm⁻¹
 $T = 293$ (2) K
 $0.1 \times 0.1 \times 0.1$ mm

Data collection

Enraf–Nonius CAD4
 diffractometer
 Absorption correction: ψ scan
 (North *et al.*, 1968)
 $T_{\min} = 0.35$, $T_{\max} = 0.46$
 2114 measured reflections

657 independent reflections
 644 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.082$
 2 standard reflections
 frequency: 120 min
 intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.025$
 $wR(F^2) = 0.059$
 $S = 0.92$
 657 reflections
 70 parameters
 4 restraints

$\Delta\rho_{\max} = 0.57$ e Å⁻³
 $\Delta\rho_{\min} = -0.49$ e Å⁻³
 Absolute structure: Flack (1983),
 123 Friedel pairs
 Flack parameter: -0.03 (3)

Table 1

Selected bond angles (°).

$\text{O4B}^i-\text{Fe2}-\text{O1}^{ii}$	89.8 (8)	$\text{O3}-\text{P}-\text{O4A}$	115.1 (3)
--	----------	---------------------------------	-----------

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

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *SHELXL97*.

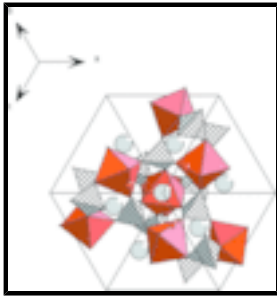
Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BR2076).

References

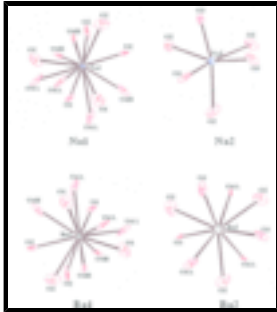
- Battle, P. D., Cheetham, A. K., Harrison, W. T. A. & Long, G. J. (1986). *J. Solid State Chem.* **62**, 16–25.
 Battle, P. D., Gibb, T. C., Nixon, S. & Harrison, W. T. A. (1988). *J. Solid State Chem.* **75**, 21–29.
 Baur, W. H. (1974). *Acta Cryst.* **B30**, 1195–1215.
 Brandenburg, K. (1998). *DIAMOND*. University of Bonn, Germany.
 Enraf–Nonius (1994). *CAD-4 EXPRESS*. Enraf–Nonius, Delft, The Netherlands.
 Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.
 Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.
 Moffat, J. B. (1978). *Catal. Rev. Sci. Eng.* **18**, 199–258.
 North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* **A24**, 351–359.
 Padhi, A., Nanjundaswamy, K. & Goodenough, J. (1997). *J. Electrochem. Soc.* **144**, 1188–1194.
 Shannon, R. D. (1976). *Acta Cryst.* **A32**, 751–767.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
 Zemmann, A. & Zemmann, J. (1957). *Acta Cryst.* **10**, 409–413.

4 4 . & 3# !" # # # ! + " # # %
 # ! \$! # # 3 #? 0 C # \$ # C \$!
 + \$! # ' F? # ! # # + \$ \$ / + ! # F #
 + + + \$ + # ! " ! * !!% \$ # 7 #
 @ ! " ! \$! !% ! \$!% # # 0
 ! \$ " # #

/ 1 # 2 \$ + ! # % # \$ # # \$ \$ + # %
 \$ D!! \$ + # !!%



2 D 9 ! #



2 \$ / " \$ 0 # 1 + \$
 G ! " !

0 1 2) 3 .
 B 8 ' 4
 ? .
 C !! % \$! E)
 B ' (' 8 ;
 B ' (' 8 ;
 B ' (' 8 ;
 I B ' L
 N B ' L

B 4
 B 4
 * B . ' . & ^ \$
 & I #
 J B ((. ;
 ? !! \$ \$!
 K B ' 5 . L
 M B (^ \$ \$
 B ' . A
) \$ 7

