Mg2—O2^{v}	2,034 (8)	Na3—O1^{x}	2,287 (7)
Mg2—O7	2,148 (7)	Na3—O4^{x}	2,854 (8)
Mg2—O8^{vi}	2,167 (7)	Na3—O6	2,852 (9)
Mg2—O10	2,056 (8)	Na3—O6^{ii}	2,327 (7)
Mg2—O11^{v}	2,488 (8)	Na3—O7^{iii}	2,606 (9)
Mg3—O4	1,970 (7)	Na3—O8^{x}	2,444 (9)
Mg3—O5	1,971 (8)	Na3—O11	2,600 (10)
Mg3—O9	2,189 (8)	Na3—O12^{iii}	2,324 (9)
O4—P1—O5^{i}	108,1 (4)	O8—Mg1—O11	113,8 (3)
O4—P1—O8	106,4 (4)	O1^{iv}—Mg2—O2^{v}	172,3 (3)
O4—P1—O10	111,2 (4)	O1^{iv}—Mg2—O7	86,5 (3)
O5^{i}—P1—O8	108,7 (4)	O1^{iv}—Mg2—O8^{vi}	91,6 (3)
O5^{i}—P1—O10	109.9 (4)	O1^{iv}—Mg2—O10	94,7 (3)
O8—P1—O10	112,4 (5)	O1^{iv}—Mg2—O11^{v}	87,7 (3)
O2—P2—O3	109,4 (4)	O2^{v}—Mg2—O7	94,7 (3)
O2—P2—O7	108,0 (4)	O2^{v}—Mg2—O8^{vi}	86,4 (3)
O2—P2—O12	112,1 (4)	O2^{v}—Mg2—O10	92,5 (3)
O3—P2—O7	109,2 (4)	O2^{v}—Mg2—O11^{v}	85,3 (3)
O3—P2—O12	107,9 (4)	O7—Mg2—O8^{vi}	173,5 (3)
O7—P2—O12	110,1 (4)	O7—Mg2—O10	101,0 (3)
O1—P3—O6	110,1 (4)	O7—Mg2—O11^{v}	73,1 (3)
O1—P3—O9	108,1 (4)	O8^{vi}—Mg2—O10	85,3 (3)
O1—P3—O11	111,1 (4)	O8^{vi}—Mg2—O11^{v}	100,6 (3)
O6—P3—O9	108,4 (4)	O10—Mg2—O11^{v}	173,5 (3)
O6—P3—O11	108,2 (4)	O4—Mg3—O5	163,7 (4)
O9—P3—O11	111,0 (5)	O4—Mg3—O9	85,2 (3)
O3—Mg1—O6^{ii}	163,8 (3)	O4—Mg3—O9^{i}	96,0 (3)
O3—Mg1—O7^{iii}	89,4 (3)	O4—Mg3—O12^{v}	95,1 (3)
O3—Mg1—O8	86,8 (3)	O5—Mg3—O9	88,5 (3)
O3—Mg1—O11	101,2 (3)	O5—Mg3—O9^{i}	87,5 (3)
O6^{ii}—Mg1—O7^{iii}	87,4 (3)	O5—Mg3—O12^{v}	99,4 (3)
O6^{ii}—Mg1—O8	92,2 (3)	O9—Mg3—O9^{i}	169,3 (4)
O6^{ii}—Mg1—O11	94,0 (3)	O9—Mg3—O12^{v}	85,5 (3)
O7^{iii}—Mg1—O8	164,7 (3)	O9^{i}—Mg3—O12^{v}	104,9 (3)
O7^{iii}—Mg1—O11	81,5 (3)		

Codes de symétrie: (i) $\frac{1}{2}-x, 1-y, z-\frac{1}{2}$; (ii) $\frac{3}{2}-x, 1-y, z-\frac{1}{2}$; (iii) $\frac{1}{2}+x, \frac{1}{2}-y, 1-z$; (iv) $1-x, y-\frac{1}{2}, \frac{1}{2}-z$; (v) $x-\frac{1}{2}, \frac{1}{2}-y, 1-z$; (vi) $x-\frac{1}{2}, \frac{1}{2}-y, -z$; (vii) $\frac{1}{2}-x, 1-y, \frac{1}{2}+z$; (viii) $x, y, z-1$; (ix) $\frac{1}{2}+x, \frac{1}{2}-y, -z$; (x) $\frac{3}{2}-x, 1-y, \frac{1}{2}+z$.

La collecte et la réduction des données: *AFC/MSC Diffractometer Control Program* (Rigaku Corporation, 1991). La solution de la structure: *TEXSAN* (Molecular Structure Corporation, 1985). L'affinement de la structure: *RSFLS*-4 dans *UNICS* (Sakurai, 1971). Les distances interatomiques et les angles: *CCPC* (Kawamura & Kawahara, 1980). La synthèse de Fourier: *RSSFR*-5 dans *UNICS* (Sakurai, 1971). Le graphique: *ORTEP*II (Johnson, 1971). L'impression des tableaux de F_o et de σF_o: *LISTHKL* (Yamakawa & Kawahara, 1994).

Les auteurs remercient à Monsieur J. T. Iiyama, professeur honoraire de l'Université de Tokio, pour les conseils qu'il nous a donnés pendant ce travail. Les intensités des réflections ont été mesurées au laboratoire de rayons X de l'Université d'Okayama, Japon.

Des documents complémentaires concernant cette structure peuvent être obtenus à partir des archives électroniques de l'UICr (Référence: DU1170). Les processus d'accès à ces archives est donné au dos de la couverture.

Références

Ben Amara, M., Vlasse, M., Olazcuaga, R., Le Flem, G. & Hagenmuller, P. (1983). *Acta Cryst.* C**39**, 936–939.

Brown, I. D. & Wu, K. K. (1976). *Acta Cryst.* B**32**, 1957–1959.

Ghorbel, A., d'Yvoire, F. & Dorémieux-Morin, C. (1974). *Bull. Soc. Chim. Fr.* pp. 1239–1242.

Johnson, C. K. (1971). *ORTEP*II. Rapport ORNL-3794, revisé. Oak Ridge National Laboratory, Tennessee, EU.

Kawamura, K. & Kawahara, A. (1980). *CCPC. Calculation of Coordination Polyhedra.* Communication Privée.

Molecular Structure Corporation (1985). *TEXSAN. TEXRAY Structure Analysis Package.* MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, EU.

Rigaku Corporation (1991). *AFC/MSC Diffractometer Control System.* Rigaku Corporation, Tokio, Japon.

Sakurai, T. (1971). Editeur. *Universal Crystallographic System.* Société Cristallographique de Japon, Tokio, Japon.

Takano, T., Tanaka, N. & Kusunoki, M. (1973). *ABSC. Absorption Correction.* Publication of the Institute for Protein Research, Osaka Université, Japon.

Yamakawa, J. & Kawahara, A. (1994). *LISTHKL. Program for F_o and F_c Tables.* Earth Science Report, Vol. 1. Université Okayama, Japon.

Yamakawa, J., Yamada, T. & Kawahara, A. (1994). *Acta Cryst.* C**50**, 986–988.

Acta Cryst. (1997). C**53**, 1735–1738

Mixed $Ba_{5.24}Sr_{0.76}Mg_7F_{26}$

FRANK KUBEL, HANS HAGEMANN AND HANS BILL

Département de Chimie Physique, Université de Genève, 30, Quai E. Ansermet, CH-1211 Genève 4, Switzerland. E-mail: frank.kubel@chiam.unige.ch

(*Received 25 November 1996; accepted 7 July 1997*)

Abstract

In orthorhombic $Ba_6Mg_7F_{26}$, the Ba^{2+} ion can be partially replaced by Sr^{2+} to form a mixed, disordered barium strontium magnesium fluoride. This new compound has a refined composition of $Ba_{5.24(4)}Sr_{0.76(4)}Mg_7F_{26}$. The volume decreases after the partial substitution from 1074.64 (10) to 1064.31 (11) Å^3. The structure has two barium sites, Ba1 on Wyckoff site 8*l* with C_s symmetry and a coordination number of 12+1, and Ba2 on site 4*j* with C_{2v} symmetry and a coordination number of 12; only the Ba^{2+} on site 4*j* is partially replaced by Sr^{2+}. The distorted octahedral fluoride environment around magnesium shows a tendency to become more irregular in the strontium-substituted compound.

Comment

During our study of rare-earth doped barium halide-containing materials (Kubel, Hagemann & Bill, 1996*a*,*b*), we became particularly interested in a low-symmetry barium environment and the possibilities for substitution of this element for use in optical applications. The *f*–*f* transitions of rare earth ions introduced into inorganic host materials are very sensitive to modifications in the local environment. Modifications can be brought about either by application of external pressure, which allows this type of compound to be used as a

Acta Crystallographica Section C
ISSN 0108-2701 © 1997

pressure indicator, or by creating a chemical pressure when some of the ions in the host material are substituted by ions of a slightly different ionic radius.

A needle-shaped crystal with (100) and (110) faces was selected for X-ray diffraction measurements. The optical indicatrix is oriented parallel to the main crystal faces and the crystal shows sharp extinction in polarized light. Analysis of the X-ray extinction shows no change from the parent structure with space group *Immm*. The starting model was taken from Kubel, Hagemann & Bill (1997*a*). Partially standardized (Gelato & Parthé, 1987) atomic positions and displacement parameters are available in the archived CIF, and selected interatomic distances around the metal ions are given in Table 1. Residual electron density was found close (~1.3 Å) to Ba1.

Analysis of the decrease of the unit-cell volume is a useful tool in estimating the amount of substitution of Sr^{2+} for Ba^{2+}. For this purpose, lattice parameters obtained from crystals with similar shapes and sizes (thus similar absorption values), and for similar sets of 2θ values ($2\theta > 80°$) were compared. For the solid solution $Ba_{1-\delta}Sr_\delta MgF_4$, a volume change of ~10±2% for complete substitution was found (Kubel, Hagemann & Bill, 1997*b*). For the title compound, a volume change of ~1% suggests replacement of *ca* 10% of the Ba^{2+} ions, if a linear relation to the volume change is assumed. This leads to a sample with composition $Ba_{5.4}Sr_{0.6}Mg_7F_{26}$. The estimated composition is close to the refined values of $Ba_{5.2}Sr_{0.8}Mg_7F_{26}$. The refined composition is different from that expected from the Ba/Sr ratio in the reaction mixture ($Ba_{4.5}Sr_{1.5}Mg_7F_{26}$). A complete replacement of Ba by Sr was unsuccessful under synthetic conditions similar to those used to prepare the title compound.

Fig. 1. A projection of the structure along [100]. The alkaline earth ions shown as spheres are located in the cavities of the MgF_6 network shown by the octahedra. The rutile chains lie along the *a* axis.

The structure of $Ba_6Mg_7F_{26}$ comprises perovskite-like blocks and rutile-related parts (see Fig. 1). Two barium sites, Ba1 on Wyckoff site 8*l* with C_s symmetry and a coordination number of 12+1, and Ba2 on site 4*j* with C_{2v} symmetry and a coordination number of 12, are present in the title structure (see Fig. 2). Both alkaline earth ions are located slightly off-centre in an approximately regular cube of fluoride ions. Substitution by the smaller Sr^{2+} was found to be rather selective. The Ba2 4*j* site is partially (~30%) substituted by Sr^{2+} ions. When replaced, the 4+2 short Ba/Sr—F distances decrease by approximately 0.042 (3) Å. The six longer distances show a slight increase or remain unchanged. Only small variations in the metal–fluoride distances were found around Ba1, indicating further that under the given synthetic conditions, no substitution takes place on this site. The partial substitution of mainly Wyckoff site

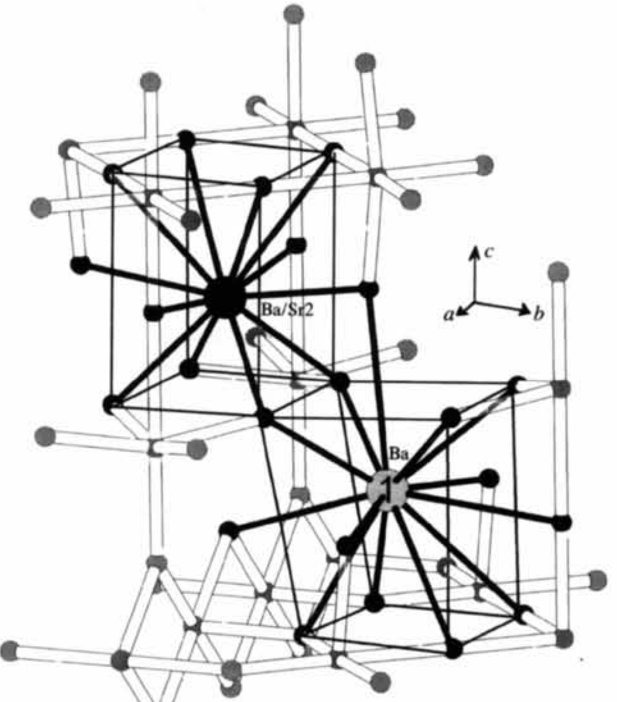

Fig. 2. The local environment around the alkaline earth ions. The coordination number of Ba1 is 12+1 and that of Ba/Sr2 is 12.

4*j* may be explained by geometric considerations. The average Ba—F distance around Ba1 is 2.954 Å, whereas that around Ba2 is 2.809 Å. The smaller Sr^{2+} ion appears to prefer to substitute the smaller cavity.

A further distortion of the irregular Mg—F octahedra is found. Distances around Mg1 range from 1.959 (3) to 2.280 (7) Å [1.960 (1) to 2.274 (3) Å in $Ba_6Mg_7F_{26}$] and around Mg2 from 1.915 (4) to 2.051 (5) Å [1.926 (2) to 2.075 (2) Å in $Ba_6Mg_7F_{26}$]. The octahedra around Mg3 and Mg4 are more regular.

Experimental

Crystals of $Ba_{1-\delta}Sr_{\delta}Mg_7F_{26}$ can been obtained for small values of δ only by slow cooling of an LiF flux containing the SrF_2/BaF_2–MgF_2 mixture. The crystals under study were obtained by heating 1.5 mol BaF_2, 0.5 mol SrF_2 and 3 mol MgF_2 together with 6 mol LiF as flux or mineralizer in a platinum crucible in air. The sample was cooled for 50 h from nominally 1203 K to 973 K. Needle- and plate-shaped crystals with well defined crystal faces could be selected from the product. Analysis of the unit-cell parameters for samples of both shapes show that they have the same composition.

Crystal data

$Ba_{5.24}Sr_{0.76}Mg_7F_{26}$
M_r = 1450.35
Orthorhombic
Immm
a = 5.8346 (3) Å
b = 12.0877 (8) Å
c = 15.0908 (9) Å
V = 1064.31 (11) Å^3
Z = 2
D_x = 4.523 Mg m^{-3}
D_m not measured

Cu $K\alpha$ radiation
λ = 1.54183 Å
Cell parameters from 25 reflections
θ = 49.6–56.2°
μ = 80.593 mm^{-1}
T = 293 K
Needle
0.420 × 0.034 × 0.020 mm
Colourless

Data collection

Enraf–Nonius CAD-4 four-circle diffractometer
ω–2θ scans
Absorption correction: analytical by integration (*Xtal LSABS*; Blanc, Schwarzenbach & Flack, 1991)
$T_{\min}$ = 0.033, $T_{\max}$ = 0.382
4559 measured reflections
658 independent reflections

658 reflections with $F > 3\sigma(F)$
$R_{\rm int}$ = 0.022
$\theta_{\max}$ = 74.99°
$h = -7 \rightarrow 6$
$k = -15 \rightarrow 15$
$l = -18 \rightarrow 18$
2 standard reflections
frequency: 30 min
intensity decay: 5%

Refinement

Refinement on F
R = 0.031
wR = 0.028
S = 3.787
654 reflections
68 parameters
Weighting scheme based on measured e.s.d.'s
$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max}$ = 1.23 e Å^{-3}
$\Delta\rho_{\min}$ = −3.22 e Å^{-3}
Extinction correction: Zachariasen (1969)
Extinction coefficient: 1079 (82)
Scattering factors from *International Tables for X-ray Crystallography* (Vol. IV)

Table 1. *Selected geometric parameters (Å)*

$Ba1^{i}$—$F1^{ii}$	2.607 (3)	$Mg1^{i}$—$F1^{x}$	1.959 (3)
$Ba1^{i}$—$F1^{iii}$	2.607 (3)	$Mg1^{i}$—$F1^{i}$	1.959 (3)
$Ba1^{i}$—$F1^{iv}$	2.778 (3)	$Mg1^{i}$—$F1^{xiii}$	1.959 (3)
$Ba1^{i}$—$F1^{i}$	2.778 (3)	$Mg1^{i}$—$F1^{iv}$	1.959 (3)
$Ba1^{i}$—$F3^{v}$	2.814 (3)	$Mg1^{i}$—$F6^{i}$	1.966 (6)
$Ba1^{i}$—$F3^{iii}$	2.814 (3)	$Mg1^{i}$—$F7^{i}$	2.280 (7)
$Ba1^{i}$—$F4^{vi}$	2.9844 (9)	$Mg2^{xii}$—$F4^{xii}$	1.915 (4)
$Ba1^{i}$—$F4^{iii}$	2.9844 (9)	$Mg2^{xii}$—$F4^{iii}$	1.915 (4)
$Ba1^{i}$—$F5^{iii}$	3.0479 (16)	$Mg2^{xii}$—$F3^{iii}$	1.957 (5)
$Ba1^{i}$—$F7^{i}$	3.1536 (7)	$Mg2^{xii}$—$F3^{xii}$	1.957 (5)
$Ba1^{i}$—$F2^{iii}$	3.214 (4)	$Mg2^{xii}$—$F2^{iii}$	2.051 (5)
$Ba1^{i}$—$F2^{v}$	3.214 (4)	$Mg2^{xii}$—$F2^{xii}$	2.051 (5)
$Ba1^{i}$—$F4^{i}$	3.411 (4)	$Mg3^{xiv}$—$F5^{xiv}$	1.953 (5)
$Ba2^{vii}$—$F4^{viii}$	2.630 (5)	$Mg3^{xiv}$—$F5^{iii}$	1.953 (5)
$Ba2^{vii}$—$F4^{iii}$	2.630 (5)	$Mg3^{xiv}$—$F3^{iii}$	1.985 (4)
$Ba2^{vii}$—$F1^{ix}$	2.630 (3)	$Mg3^{xiv}$—$F3^{xiv}$	1.985 (4)
$Ba2^{vii}$—$F1^{iv}$	2.630 (3)	$Mg3^{xiv}$—$F6^{iii}$	2.001 (5)
$Ba2^{vii}$—$F1^{x}$	2.630 (3)	$Mg3^{xiv}$—$F6^{xiv}$	2.001 (5)
$Ba2^{vii}$—$F1^{vii}$	2.630 (3)	$Mg4^{xi}$—$F7^{xv}$	1.946 (6)
$Ba2^{vii}$—$F7^{vii}$	2.9345 (7)	$Mg4^{xi}$—$F7^{i}$	1.946 (6)
$Ba2^{vii}$—$F7^{i}$	2.9345 (7)	$Mg4^{xi}$—$F2^{xi}$	1.980 (5)
$Ba2^{vii}$—$F2^{iii}$	3.016 (4)	$Mg4^{xi}$—$F2^{v}$	1.980 (5)
$Ba2^{vii}$—$F2^{viii}$	3.016 (4)	$Mg4^{xi}$—$F2^{iii}$	1.980 (5)
$Ba2^{vii}$—$F2^{xi}$	3.016 (4)	$Mg4^{xi}$—$F2^{xvi}$	1.980 (5)
$Ba2^{vii}$—$F2^{xii}$	3.016 (4)		

Symmetry codes: (i) $\frac{1}{2}+x, \frac{1}{2}+y, \frac{1}{2}+z$; (ii) $1-x, 1-y, 1-z$; (iii) $x, 1-y, 1-z$; (iv) $\frac{1}{2}-x, \frac{1}{2}+y, \frac{1}{2}+z$; (v) $1-x, 1-y, 1+z$; (vi) $1+x, 1-y, 1-z$; (vii) $x-\frac{1}{2}, \frac{1}{2}+y, \frac{1}{2}+z$; (viii) $-x, y, 1-z$; (ix) $x-\frac{1}{2}, \frac{1}{2}-y, \frac{1}{2}+z$; (x) $\frac{1}{2}-x, \frac{1}{2}-y, \frac{1}{2}+z$; (xi) $x, y, 1+z$; (xii) $-x, 1-y, 1+z$; (xiii) $\frac{1}{2}+x, \frac{1}{2}-y, \frac{1}{2}+z$; (xiv) $x, 1+y, 1+z$; (xv) $\frac{1}{2}+x, \frac{1}{2}-y, \frac{3}{2}-z$; (xvi) $1-x, y, 1-z$.

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989). Cell refinement: *CELDIM* in *CAD*-4 *Software*. Data reduction: *Xtal*3.2 *REFCAL*, *LSABS* and *SORTRF* (Hall, Flack & Stewart, 1992). Program(s) used to solve structure: *Xtal*3.2 *GENTAN*. Program(s) used to refine structure: *Xtal*3.2 *CRYLSQ*. Molecular graphics: *ATOMS* (Dowty, 1989). Software used to prepare material for publication: *Xtal*3.2 *BONDLA* and *CIFIO*.

This work was supported by the Swiss National Science Foundation and the Swiss Optics Priority Program I.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: BR1171). Services for accessing these data are described at the back of the journal.

References

Blanc, E., Schwarzenbach, D. & Flack, H. D. (1991). *J. Appl. Cryst.* **24**, 1035–1041.
Dowty, E. (1989). *ATOMS. A Computer Program for Displaying Atomic Structures.* Shape Software, 521 Hidden Valley Road, Kingsport, TN 37663, USA.
Enraf–Nonius (1989). *CAD*-4 *Software*. Version 5. Enraf–Nonius, Delft, The Netherlands.
Gelato, L. M. & Parthé, E. (1987). *J. Appl. Cryst.* **20**, 139–143.
Hall, S. R., Flack, H. D. & Stewart, J. M. (1992). Editors. *Xtal*3.2 *Reference Manual.* Universities of Western Australia, Australia, Geneva, Switzerland, and Maryland, USA.
Kubel, F., Hagemann, H. & Bill, H. (1996*a*). *Z. Anorg. Allg. Chem.* **622**, 343–347.
Kubel, F., Hagemann, H. & Bill, H. (1996*b*). *Z. Anorg. Allg. Chem.* **622**, 1374–1380.
Kubel, F., Hagemann, H. & Bill, H. (1997*a*). *Z. Anorg. Allg. Chem.* **623**, 573–578.

Kubel, F., Hagemann, H. & Bill, H. (1997*b*). *Mater. Res. Bull.* **32**, 263–269.
Zachariasen, W. H. (1969). *Acta Cryst.* A**25**, 102.

Acta Cryst. (1997). C**53**, 1738–1739

A New Zinc Pyrovanadate, $Zn_3(OH)_2V_2O_7.2H_2O$, from X-ray Powder Data

Peter Y. Zavalij, Fan Zhang and M. Stanley Whittingham

Materials Research Center, State University of New York at Binghamton, Binghamton, NY 13902-6016, USA. E-mail: zavalij@binghamton.edu

(*Received 14 April 1997; accepted 30 June 1997*)

Abstract

Hydrothermally prepared zinc dihydroxide divanadate dihydrate crystallizes in the trigonal system (space group $P\bar{3}m1$). Its structure was solved *ab initio* from conventional X-ray powder data. Zn atoms occupy three of four octahedral sites in a close-packed layer of O atoms. These layers are connected by pyrovanadate groups and form a porous framework. Relatively large cavities are filled by water molecules.

Comment

Recently, mild hydrothermal reactions driven by template cations such as tetramethylammonium (Whittingham *et al.*, 1995) and/or hydrated transition metals were successfully used to obtain metastable vanadium oxide phases. These compounds, with relatively open frameworks, are of particular interest as cathode materials in lithium batteries and electrochromic devices. We have also shown that the tetramethylammonium ion is capable of providing a range of new vanadium oxides, $Li_xV_{2-y}O_{4-y}.H_2O$ (Chirayil, Zavalij & Whittingham, 1996*a*) and $Li_xV_{2-y}O_{4-y}$ (Chirayil, Zavalij & Whittingham, 1996*b*), and their intercalates $[N(CH_3)_4]V_4O_{10}$ (Zavalij, Whittingham, Boylan, Pecharskii & Jacobson, 1996), $[N(CH_3)_4]V_3O_7$ (Zavalij, Chirayil & Whittingham, 1997). This work presents the crystal structure of a new zinc hydroxide pyrovanadate, which was found during systematic investigations of the hydrothermal interactions in the system $ZnCl_2–V_2O_5–[N(CH_3)_4]OH$.

The title structure is built up of zinc oxide layers which are kept apart by pyrovanadate columns (Fig. 1). This brucite type of layer is formed by close-packed terminal O atoms of pyrovanadate and hydroxide groups. The Zn atoms occupy three of four octahedral sites. The remaining site is surrounded by pyrovanadate tetrahedra. The OH group forms a hydrogen bond (Table 1) to the water molecules that fill cavities in the porous framework. The size of these cavities is much greater than is required. Therefore, the water molecules are disordered around the site $\frac{2}{3}, \frac{1}{3}, \frac{1}{2}$ and are able to make strong hydrogen bonds. The two distances $Ow\cdots O2$ of length 2.84 (2) Å indicate the presence of two hydrogen bonds formed by H atoms of the water molecules.

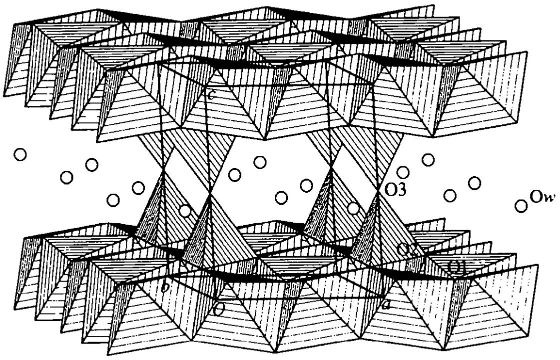

Fig. 1. Polyhedral representation of $Zn_3(OH)_2V_2O_7.2H_2O$.

The structure of the zinc hydroxide pyrovanadate is very similar to that of thallium pyrovanadate, $Tl_4V_2O_7$ (Jouanneaux, Joubert, Evain & Ganne, 1992), where the V_2O_7 group is at the same position as in the zinc compound and two Tl atoms occupy the positions of the water molecule (O*w*) and the hydroxide group (O1). The Zn site is unoccupied. The copper pyrovanadate compound $Cu_3(OH)_2V_2O_7.2H_2O$, with the same stoichiometry as the title compound (Basso, Palenzona & Zefiro, 1988; Lafontaine, Le-Bail & Ferey, 1990), is almost identical to the zinc compound. The lattice of the copper compound (space group *C*2/*m*) is derived from the hexagonal lattice of the zinc compound by a

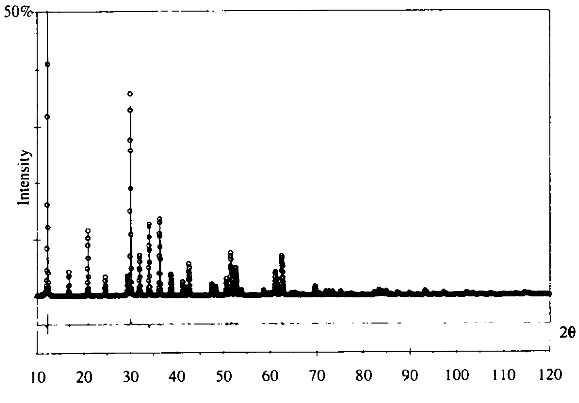

Fig. 2. Comparison of observed (circles) and calculated (solid line) intensities for $Zn_3(OH)_2V_2O_7.2H_2O$. The difference pattern appears below.