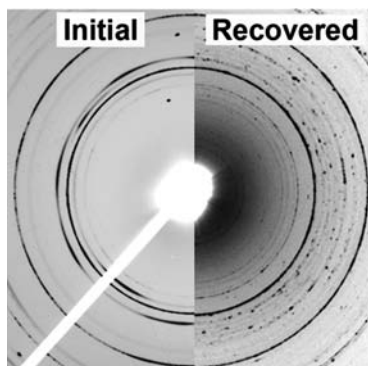


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### Regular Articles

#### Formation of scandium carbides and scandium oxycarbide from the elements at high-(*P*, *T*) conditions

Erick A. Juarez-Arellano, Björn Winkler, Lkhamsuren Bayarjargal, Alexandra Friedrich, Victor Milman, Daniel R. Kammler, Simon M. Clark, Jinyuan Yan, Monika Koch-Müller, Florian Schröder and Miguel Avalos-Borja  
Page 975

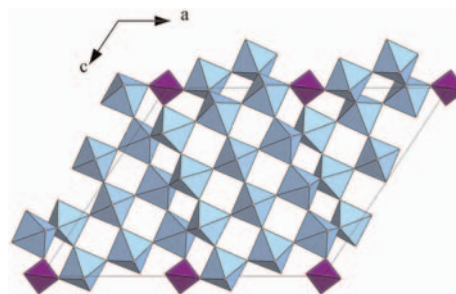


Selected images recorded with a MAR345 image plate detector show the reaction of  $\alpha$ -Sc and graphite at high-(*P*, *T*) conditions. Left: mixture of  $\alpha$ -Sc and graphite. Right: recovered sample after laser heated the diamond anvil cell.

### Regular Articles—Continued

#### Electrochemical Li insertion studies on $\text{WNb}_{12}\text{O}_{33}$ —A shear $\text{ReO}_3$ type structure

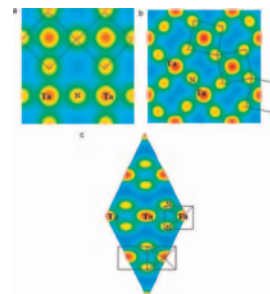
D. Saritha, V. Pralong, U.V. Varadaraju and B. Raveau  
Page 988



The projected structure can be described as  $3 \times 4 \times \infty$   $\text{ReO}_3$  type blocks of  $\text{NbO}_6$  octahedra sharing corners, joined with identical blocks via tetrahedrally coordinated tungsten atoms.

#### Potential existence of post-perovskite nitrides; DFT studies of $\text{ThTaN}_3$

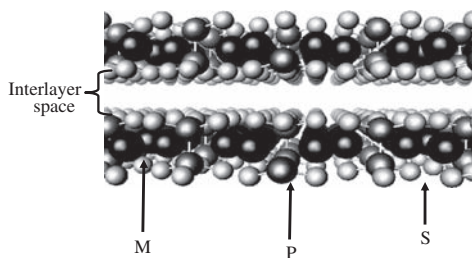
Samir F. Matar and Gérard Demazeau  
Page 994



$\text{ThTaN}_3$ : Projected charge density (for 4fu) onto basal plane: (a) cubic perovskite, (b) orthorhombic perovskite and (c) post-perovskite. Red, green and blue areas are relevant to strong, medium and low localization of density.

#### Synthesis and characterization of $\text{MnPS}_3$ for hydrogen sorption

N. Ismail, Y.M. Temerk, A.A. El-Meligi, M.A. Badr and M. Madian  
Page 984

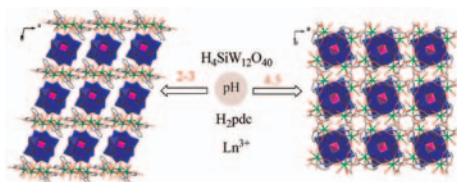


Atomic building of  $\text{MPS}_3$ .

### Syntheses, structures and properties of 3D inorganic–organic hybrid frameworks constructed from lanthanide polymer and Keggin-type tungstosilicate

Yuanzhe Gao, Yanqing Xu, Zhangang Han, Chunhong Li, Fengyun Cui, Yingnan Chi and Changwen Hu

Page 1000



Two types of new inorganic–organic hybrid frameworks through incorporation of Keggin-type heteropolyanion  $[\text{SiW}_{12}\text{O}_{40}]^{4-}$  within the voids of lanthanides-pdc network as pillars or guests under hydrothermal condition were successfully assembled. Solid-state properties of compounds **1** and **2a** such as thermal stability and photoluminescence have been further investigated.

### Degree of order and redox balance in B-site ordered double-perovskite oxides, $\text{Sr}_2\text{MMoO}_{6-\delta}$ ( $M = \text{Mg, Mn, Fe, Co, Ni, Zn}$ )

S. Vasala, M. Lehtimäki, Y.H. Huang, H. Yamauchi, J.B. Goodenough and M. Karppinen

Page 1007

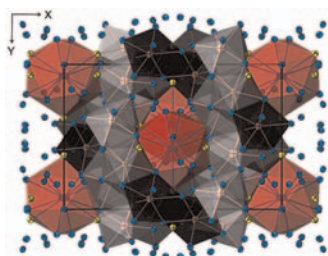


A series of  $\text{Sr}_2\text{MMoO}_{6-\delta}$  compounds with  $M = \text{Mg, Mn, Fe, Co, Ni}$  and  $\text{Zn}$  is investigated for their crystal structure, redox stability and precise oxygen content in order to address systematically the questions concerning the cation (dis)order, oxygen (non)stoichiometry and valence mixing in B-site ordered double-perovskite oxides.

### On phase equilibria and crystal structures in the systems Ce–Pd–B and Yb–Pd–B. Physical properties of $\text{R}_2\text{Pd}_{13.6}\text{B}_5$ ( $R = \text{Yb, Lu}$ )

Oksana Sologub, Peter Rogl, Leonid Salamakha, Ernst Bauer, Gerfried Hilscher, Herwig Michor and Gerald Giester

Page 1013

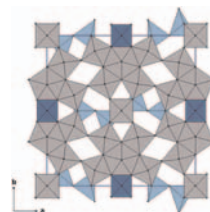


Crystal structure of  $\text{CePd}_8\text{B}_{2-x}$ .

### $\text{V}_{2.38}\text{Nb}_{10.7}\text{O}_{32.7}$ : A $\text{V}_2\text{O}_5$ – $\text{Nb}_2\text{O}_5$ mixed oxide tunnel structure related to the tetragonal tungsten bronzes

Carina Börrnert, Wilder Carrillo-Cabrera, Paul Simon and Hubert Langbein

Page 1038

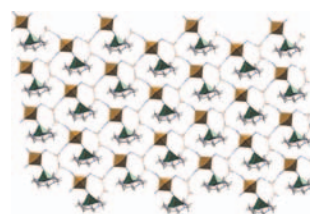


A crystal structural model for the orthorhombic compound  $\text{V}_{2.38}\text{Nb}_{10.7}\text{O}_{32.7}$ , which is known as “ $\text{V}_2\text{Nb}_9\text{O}_{27.5}$ ”, was developed by means of selected area electron diffraction, Rietveld refinement and high resolution electron microscopy. In dependence on the synthesis method the metastable compound is obtained as chain-like agglomerated nanoparticles or as more compact micro-scaled crystals.  $\text{V}_{2.38}\text{Nb}_{10.7}\text{O}_{32.7}$  is the first and only example of a compound with a TTB-type structure (space group  $Cmmm$ ) in the system  $\text{V}_2\text{O}_5$ – $\text{Nb}_2\text{O}_5$ .

### Copper(II) cyanido-bridged bimetallic nitroprusside-based complexes: Syntheses, X-ray structures, magnetic properties, $^{57}\text{Fe}$ Mössbauer spectroscopy and thermal studies

Zdeněk Trávníček, Radovan Herchel, Jiří Mikulík and Radek Zbořil

Page 1046

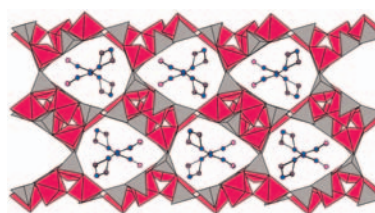


Three heterobimetallic cyano-bridged copper(II) nitroprusside-based complexes of the general compositions of  $[\text{Cu}(\text{L})\text{Fe}(\text{CN})_5\text{NO}] \cdot x\text{H}_2\text{O}$ , where  $L = N,N'$ -bis(3-aminopropyl)ethylenediamine (complex **1**), 1,3,6,9,11,14-hexaazatricyclo[12.2.1.1<sup>6,9</sup>]-octadecane (complex **2**) and  $N$ -methylethylenediamine (complex **3**), were synthesized, and fully structurally and magnetically characterized. SEM, EDS, XRD and  $^{57}\text{Fe}$  Mössbauer experiments were used for characterization of thermal decomposition products of complexes **2** and **3**.

### Structure investigation of fluorinated aluminophosphate ULM-3 Al templated by 3-methylaminopropylamine

Natasa Zabukovec Logar, Gregor Mali, Nevenka Rajic, Sanja Jevtic, Mojca Rangus, Amalija Golobic and Venceslav Kaucic

Page 1055

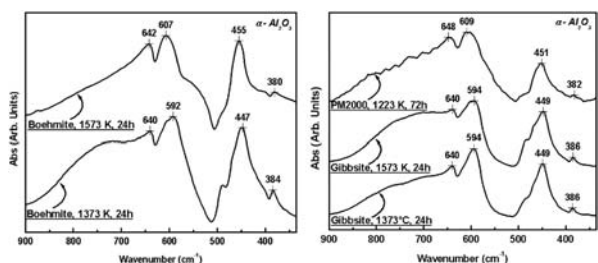


The aluminophosphate analogue of open-framework gallophosphate ULM-3 was synthesized in the presence of 3-methylaminopropylamine. The  $Pcab$  crystal symmetry and hydrogen bonding scheme was determined by single-crystal X-ray diffraction and NMR spectroscopy.

### Estimation of the intrinsic stresses in $\alpha$ -alumina in relation with its elaboration mode

A. Boumaza and A. Djelloul

Page 1063

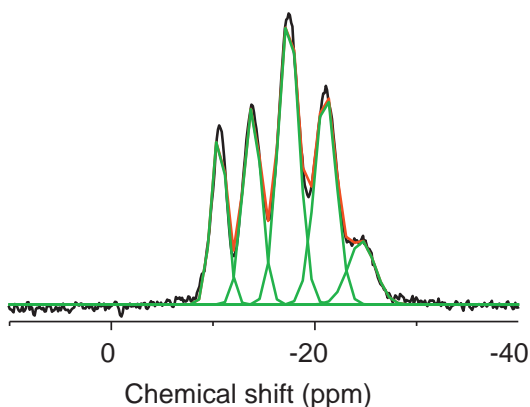


The infrared peak at  $378.7\text{ cm}^{-1}$  was used as a reference for stress free  $\alpha$ -alumina and the shift of this peak allowed to estimate intrinsic stresses, which were related to the morphology and to the specific surface area of aluminas according to their elaboration mode.

### Non-random cation distribution in hexagonal $\text{Al}_{0.5}\text{Ga}_{0.5}\text{PO}_4$

S.K. Kulshreshtha, O.D. Jayakumar and V. Sudarsan

Page 1071

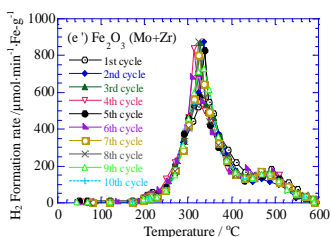


$^{31}\text{P}$  MAS NMR pattern of hexagonal  $\text{Al}_{0.5}\text{Ga}_{0.5}\text{PO}_4$  solid solution.

### Hydrogen production from water decomposition by redox of $\text{Fe}_2\text{O}_3$ modified with single- or double-metal additives

Xiaojie Liu and Hui Wang

Page 1075

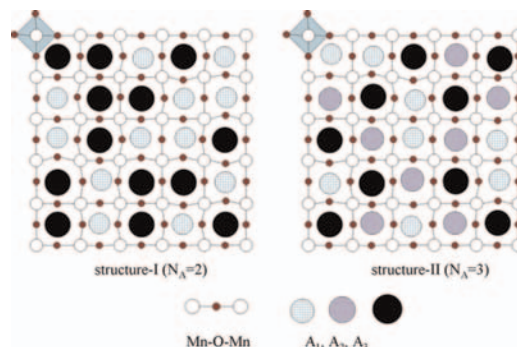


Mo+Zr additive has the best modified effect on improving the redox performances of  $\text{Fe}_2\text{O}_3:\text{H}_2$  producing temperature of  $276\text{ }^\circ\text{C}$  and hydrogen storage capacity of 4.73 wt%.

### Effects of the A-site cation number on the properties of $\text{Ln}_{5/8}\text{M}_{3/8}\text{MnO}_3$ manganites

J.A. Collado, J.L. García-Muñoz and M.A.G. Aranda

Page 1083



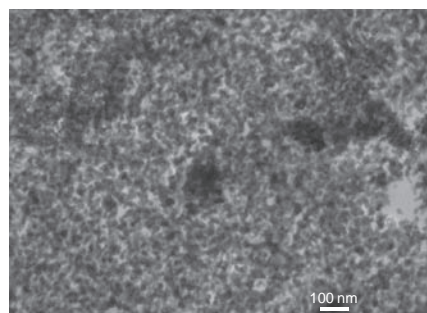
In this paper the influence of A-site cation number is shown, see attached schematic figure, on the magnetotransport properties of  $T_C$ -optimized manganites,  $\text{Ln}_{5/8}\text{M}_{3/8}\text{MnO}_3$ .

### Chemical route for formation of intermetallic $\text{Zn}_4\text{Sb}_3$ phase

A. Denoix, A. Solaiappan, R.M. Ayril, F. Rouessac and

J.C. Tedenac

Page 1090



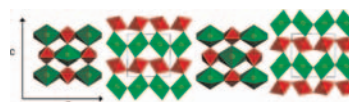
TEM observation of the  $\text{Zn}_4\text{Sb}_3$  powder synthesized by soft chemistry.

### Structural and conductivity studies of $\text{Y}_{10-x}\text{La}_x\text{W}_2\text{O}_{21}$

Anna Lashtabeg, John Bradley, Andrew Dicks,

Graeme Auchterlonie and John Drennan

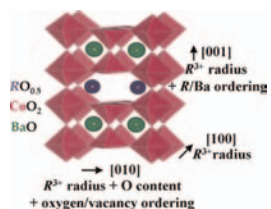
Page 1095



The solubility limit of  $\text{La}_2\text{O}_3$  in  $\text{Y}_{10}\text{W}_2\text{O}_{21}$  was found to be  $> 50\%$  after which the structure was found to change to Weberite type structure,  $\text{A}'\text{A}''\text{B}'\text{B}''\text{O}_7$ , that is closely related to the pyrochlore.

Continued

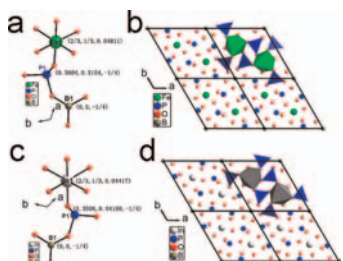
**R-site varied series of  $R\text{BaCo}_2\text{O}_{5.5}$  ( $R_2\text{Ba}_2\text{Co}_4\text{O}_{11}$ ) compounds with precisely controlled oxygen content**  
Eeva-Leena Rautama and Maarit Karppinen  
Page 1102



The entire family of carefully oxygen-adjusted  $R\text{BaCo}_2\text{O}_{5.5}$  ( $R = \text{Y}, \text{La-Ho}$ ) double-perovskite cobalt oxides is systematically studied for lattice parameters and peculiar physical properties. The results indicate  $R/\text{Ba}$  cation and oxygen/vacancy disorders for the largest  $R$  constituents with  $\text{Nd}, \text{Pr}$  and  $\text{La}$ . The physical properties are found to be sensitive even for tiny deviations from the ideal 5.5 oxygen stoichiometry.

**Synthesis and characterizations of two anhydrous metal borophosphates:  $M_2^{\text{III}}\text{BP}_3\text{O}_{12}$  ( $M = \text{Fe}, \text{In}$ )**

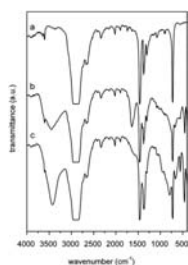
Wei-Long Zhang, Chen-Sheng Lin, Lei Geng, Ye-Yu Li, Hao Zhang, Zhang-Zhen He and Wen-Dan Cheng  
Page 1108



Two anhydrous metal borophosphates of  $M_2^{\text{III}}\text{BP}_3\text{O}_{12}$  ( $M = \text{Fe}, \text{In}$ ) have been prepared and characterized. They both crystallize in the hexagonal system, space group  $P6(3)/m$  (no. 176) and feature 3D architectures built up of the  $M_2\text{O}_9$  units and  $\text{B}(\text{PO}_4)_3$  groups via sharing the corners, but they are not isomorphic for the different crystallographically distinct atomic positions.

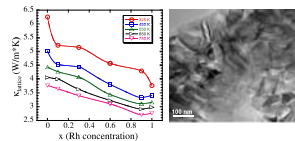
**Synthesis and selective IR absorption properties of iminodiacetic-acid intercalated MgAl-layered double hydroxide**

Lijing Wang, Xiangyu Xu, David G. Evans, Xue Duan and Dianqing Li  
Page 1114



Intercalation of iminodiacetic acid (IDA) anions in a  $\text{MgAl-NO}_3$ -layered double hydroxide host leads to an enhancement of its infrared absorbing ability for application in agricultural plastic films.

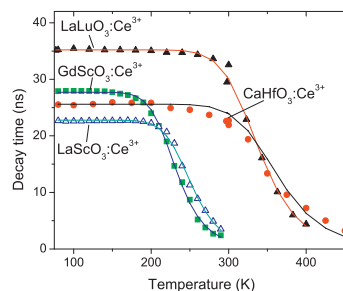
**Effects of Rh on the thermoelectric performance of the p-type  $\text{Zr}_{0.5}\text{Hf}_{0.5}\text{Co}_{1-x}\text{Rh}_x\text{Sb}_{0.99}\text{Sn}_{0.01}$  half-Heusler alloys**  
Pramathesh Maji, Nathan J. Takas, Dinesh K. Misra, Heike Gabrich, Kevin Stokes and Pierre F.P. Poudeu  
Page 1120



Significant reduction of the lattice thermal conductivity with increasing Rh concentration in the  $p$ -type  $\text{Zr}_{0.5}\text{Hf}_{0.5}\text{Co}_{1-x}\text{Rh}_x\text{Sb}_{0.99}\text{Sn}_{0.01}$  half-Heusler materials prepared by solid state reaction at 1173 K.

**Cerium luminescence in  $nd^0$  perovskites**

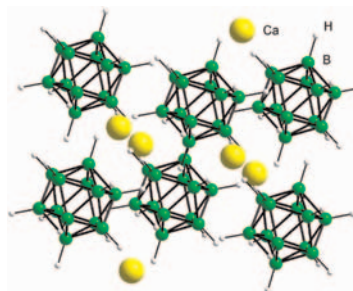
A.A. Setlur and U. Happek  
Page 1127



$\text{Ce}^{3+}$  decay times versus temperature for perovskites with  $nd^0$  B-site cations, specifically  $\text{Ca}(\text{Hf,Zr})\text{O}_3$  and  $(\text{La,Gd})\text{ScO}_3$ , is investigated in this report.

**Probing the structure, stability and hydrogen storage properties of calcium dodecahydro-closo-dodecaborate**

Vitalie Stavila, Jae-Hyuk Her, Wei Zhou, Son-Jong Hwang, Chul Kim, Leigh Anna M. Ottley and Terrence J. Udovic  
Page 1133

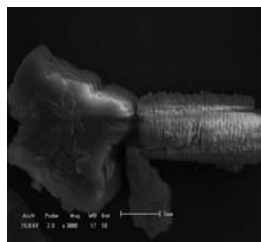


Calcium dodecahydro-closo-dodecaborate,  $\text{CaB}_{12}\text{H}_{12}$  (1), was isolated by dehydration/desolvation of  $[\text{Ca}(\text{H}_2\text{O})_7][\text{B}_{12}\text{H}_{12}] \cdot \text{H}_2\text{O}$  (2) or  $[\text{Ca}(\text{H}_2\text{O})_5(\text{MeCN})_2][\text{B}_{12}\text{H}_{12}]$  (3). The crystal structure of 1 was determined by powder X-ray diffraction and confirmed by neutron vibrational spectroscopy and first-principles calculations. Hydrogen storage properties of 1 in the presence of calcium hydride were elucidated.

**Application of Brazilian kaolinite clay as adsorbent to removal of U(VI) from aqueous solution: Kinetic and thermodynamic of cation–basic interactions**

Denis L. Guerra, Victor L. Leidens, Rúbia R. Viana and Claudio Airoidi

Page 1141

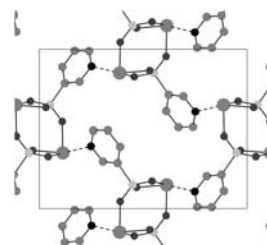


This investigation reports the use of original and modified kaolinites as alternative adsorbents. The compound N-[3-trimethoxysilylpropyl]diethylenetriamine was anchored onto Amazon kaolinite surface by heterogeneous route.

**Structural variations of Sn<sup>II</sup> pyridylphosphonates influenced by an uncommon Sn–N interaction**

Houston Perry, Jerzy Zoń, Justin Law and Abraham Clearfield

Page 1165

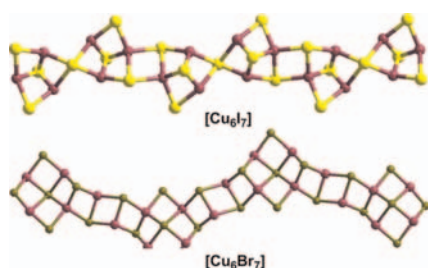


Interactions between pyridyl nitrogen atoms and Sn<sup>II</sup> affect the packing of tin phosphonate ladders in the structures of Sn<sup>II</sup> pyridylphosphonates.

**Two anionic [Cu<sub>6</sub>X<sub>7</sub>]<sup>n-</sup> (X = Br and I) chain-based organic–inorganic hybrid solids with N-substituted benzotriazole ligands**

Xia Gao, Quan-Guo Zhai, Shu-Ni Li, Rui Xia, Hai-Juan Xiang, Yu-Cheng Jiang and Man-Cheng Hu

Page 1150

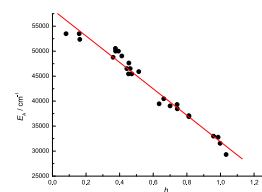


Two unprecedented anionic [Cu<sub>6</sub>X<sub>7</sub>]<sup>n-</sup> (X = Br and I) chain-based organic–inorganic hybrid solids, namely, {(HETA)[(Cu<sub>6</sub>I<sub>7</sub>)(ETA)<sub>2</sub>]<sub>n</sub> (1) and {K(Cu<sub>6</sub>Br<sub>7</sub>)(BBTH)<sub>n</sub> (2) (ETA = N-ethylbenzotriazole, HETA = protonated N-ethylbenzotriazole, BBTH = 1,6-bis(benzotriazole)-hexane) have been synthesized under solvothermal reactions and characterized.

**Prediction and assignment of site occupation and energy levels for Pb<sup>2+</sup> ions in crystal hosts**

Qiang Sun, Jing Wang and Jinsheng Shi

Page 1174

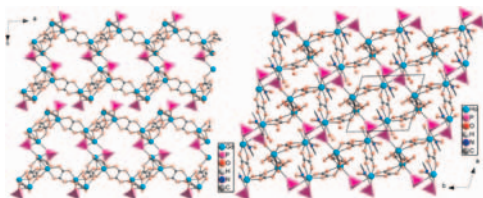


The A band energy  $E_A$  of Pb<sup>2+</sup> has linear relationship with environmental factor  $h_e$ .

**Lanthanide oxalatophosphonates with two- and three-dimensional structures**

Ting-Hai Yang, Deng-Ke Cao, Yi-Zhi Li and Li-Min Zheng

Page 1159

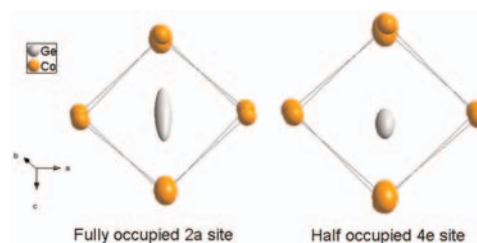


Compounds [Ln<sub>4</sub>(ox)<sub>5</sub>(2-pmpH)<sub>2</sub>(H<sub>2</sub>O)<sub>7</sub>] · 5H<sub>2</sub>O (Ln = Gd, Tb, Dy; 2-pmp = 2-pyridylmethylphosphonate) and [Ln<sub>4</sub>(ox)<sub>5</sub>(2-pmpH)<sub>2</sub>(H<sub>2</sub>O)<sub>6</sub>] · 6H<sub>2</sub>O (Ln = Ho, Yb) with 2D and 3D structures, respectively, are reported.

**Crystal structure and electronic properties of the new compounds U<sub>3</sub>Co<sub>12-x</sub>X<sub>4</sub> with X = Si, Ge**

A. Soudé, O. Tougait, M. Pasturel, D. Kaczorowski and H. Noël

Page 1180

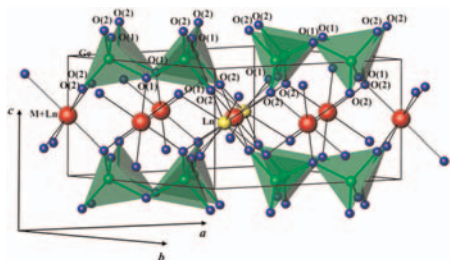


The crystal structure of the new compounds U<sub>3</sub>Co<sub>12-x</sub>X<sub>4</sub>, X = Si, Ge is a ternary ordered variant of the EuMg<sub>5.2</sub>-type with a site preference for the 4e position.

Continued

**Synthesis and crystal structure of  $Ln_2M^{2+}Ge_4O_{12}$ ,  
 $Ln$  = rare-earth element or Y;  $M$  = Ca, Mn, Zn**

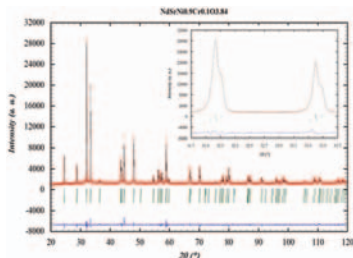
Vladimir G. Zubkov, Nadezda V. Tarakina,  
Ivan I. Leonidov, Alexander P. Tyutyunnik,  
Ludmila L. Surat, Marina A. Melkozerova,  
Elena V. Zabolotskaya and Dina G. Kellerman  
**Page 1186**



Crystal structure of  $Ln_2MGe_4O_{12}$ , where  $Ln$  = rare-earth element or Y;  $M$  = Ca, Mn, Zn.

**Investigation on the structural and electrical properties of  
 $NdSrNi_{1-x}Cr_xO_{4+\delta}$  ( $0.1 \leq x \leq 0.9$ ) system**

Manel Jammali, H. Chaker, K. Cherif and R. Ben Hassen  
**Page 1194**



The X-ray pattern of the  $x=0.1$  sample showed a shift of some Bragg reflections that was indicative of a unit cell of lower symmetry. Two distortions of the  $I4/mmm$   $K_2NiF_4$  aristotype cell to orthorhombic symmetry are known,  $Fmmm$  and  $I mmm$ , depending on which of the  $\langle 100 \rangle$  and  $\langle 110 \rangle$  sets of mirror planes and twofold axes are lost together with the fourfold axis when the symmetry is lowered.

**Rapid Communications**

**Synthesis and crystal structure of new layered  
 $BaNaSc(BO_3)_2$  and  $BaNaY(BO_3)_2$  orthoborates**

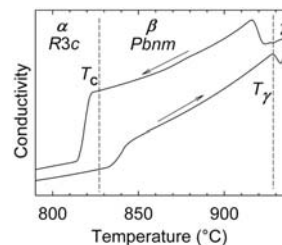
Yurii V. Seryotkin, Vladimir V. Bakakin,  
Aleksandr E. Kokh, Nadezhda G. Kononova,  
Tatyana N. Svetlyakova, Konstantin A. Kokh and  
Tatyana N. Drebushchak  
**Page 1200**



The distinctive feature of new orthoborate crystals  $BaNaSc(BO_3)_2$  and  $BaNaY(BO_3)_2$  is the combination of base building packages of two types:  $\{M^{3+}[Ba^{2+}(BO_3)_3]_2\}^+$  and  $\{M^{3+}[Na^+(BO_3)_3]_2\}^-$ , where  $M$  is Sc or Y.

**Phase transitions, electrical conductivity and chemical  
stability of  $BiFeO_3$  at high temperatures**

Sverre M. Selbach, Thomas Tybell, Mari-Ann Einarsrud  
and Tor Grande  
**Page 1205**



The structural phase transitions of multiferroic  $BiFeO_3$  are shown to first order, with discontinuous volume and electrical conductivity. Semiconductivity was found for all three polymorphs of  $BiFeO_3$ .

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