### JOURNAL OF SOLID STATE CHEMISTRY

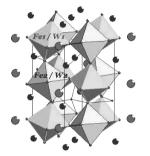
Volume 178, Number 12, December 2005

### CONTENTS

#### **Regular** Articles

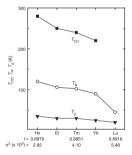
# Structural and magnetic properties of perovskite Ca<sub>3</sub>Fe<sub>2</sub>WO<sub>9</sub>

Sergey A. Ivanov, Sten Gunnar Eriksson, Roland Tellgren and Häkan Rundlöf *Page 3605* 



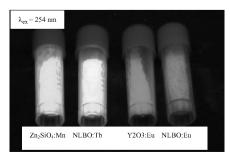
The monoclinic perovskite structure of Ca<sub>3</sub>Fe<sub>2</sub>WO<sub>9</sub>.

Structure, magnetism and transport of the perovskite manganites  $Ln_{0.5}Ca_{0.5}MnO_3$  (Ln = Ho, Er, Tm, Yb and Lu) Kenji Yoshii, Hideki Abe and Naoshi Ikeda *Page 3615* 



The values of  $T_{\rm CO}$ ,  $T_{\rm N}$ , and  $T_{\rm g}$  against the *Ln* ion for all the  $Ln_{0.5}$ Ca<sub>0.5</sub>MnO<sub>3</sub> studied (*Ln*: Ho–Lu).

#### A new promising phosphor, Na<sub>3</sub>La<sub>2</sub>(BO<sub>3</sub>)<sub>3</sub>:Ln (Ln = Eu, Tb) Zhihua Li, Jinghui Zeng, Guochun Zhang and Yadong Li Page 3624

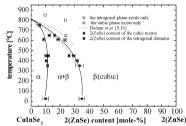


The picture of  $Na_3La_2(BO_3)_3:Ln(Ln = Tb^{3+}, Eu^{3+})$  phosphors under Mercury-free fluorescence lamp.

### **Regular** Articles—Continued

The two-phase region in  $2(ZnSe)_x(CuInSe_2)_{1-x}$  alloys and structural relation between the tetragonal and cubic phases G. Wagner, S. Lehmann, S. Schorr, D. Spemann and Th. Doering

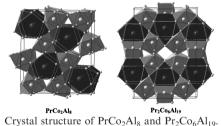
Page 3631



Two-phase region in the system  $2(\text{ZnSe})_x(\text{CulnSe}_2)_{1-x}$  for different temperatures (terminated by full lines). The bold squares represent the composition of the tetragonal phase and the bold circles that of the cubic one. According to Bodnar et al. (Inst. Phys. Conf. Ser. 152 (1997) 119) the two-phase coexistence area was found between both dotted lines.

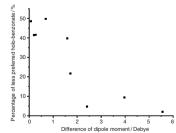
## PrCo<sub>2</sub>Al<sub>8</sub> and Pr<sub>2</sub>Co<sub>6</sub>Al<sub>19</sub>: Crystal structure and electronic properties

O. Tougait, D. Kaczorowski and H. Noël *Page 3639* 



Selective anion-exchange intercalation of isomeric benzoate anions into the layered double hydroxide [LiAl<sub>2</sub>(OH)<sub>6</sub>]Cl·H<sub>2</sub>O

Lixu Lei, Aamir Khan and Dermot O'Hare Page 3648

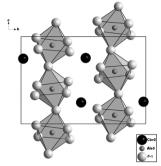


All the geometric isomers of the nine benzoate derivatives have been intercalated into  $[LiAl_2(OH)_6]Cl \cdot H_2O$  in 50% (v/v) water/ ethanol solution. Competitive intercalation studies using binary mixtures of the isomeric benzoates suggest that dipole moment may be a good general index for the preference.

# Structural investigations of $\beta$ -CaAlF<sub>5</sub> by coupling powder XRD, NMR, EPR and spectroscopic parameter calculations

M. Body, G. Silly, C. Legein, J.-Y. Buzaré, F. Calvayrac and P. Blaha

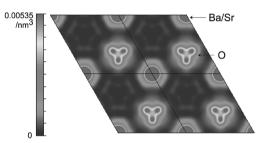
Page 3655



View of  $\beta$ -CaAlF<sub>5</sub>, exhibiting isolated chains of AlF<sub>6</sub><sup>3–</sup> octahedra sharing opposite corners.

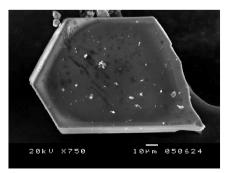
#### Structural disorder in Ba<sub>0.6</sub>Sr<sub>0.4</sub>Al<sub>2</sub>O<sub>4</sub>

Koichiro Fukuda, Tomoyuki Iwata and Takashi Orito Page 3662



Two-dimensional electron density distribution map showing positional disorder of oxygen atoms in  $Ba_{0.6}Sr_{0.4}Al_2O_4$ .

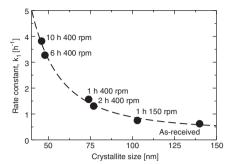
Single-crystal synthesis and structure refinement of the LiCoO<sub>2</sub>-LiAlO<sub>2</sub> solid-solution compounds: LiAl<sub>0.32</sub>Co<sub>0.68</sub>O<sub>2</sub> and LiAl<sub>0.71</sub>Co<sub>0.29</sub>O<sub>2</sub> Yasuhiko Takahashi, Norihito Kijima and Junji Akimoto *Page 3667* 



SEM photograph of a transparent  $LiAl_{0.71}Co_{0.29}O_2$  single crystal.

## Dehydrogenation kinetics of as-received and ball-milled LiAlH<sub>4</sub>

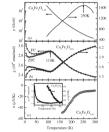
A. Andreasen, T. Vegge and A.S. Pedersen *Page 3672* 



Effect of ball milling on kinetics. Rate constants for the dehydrogenation of lithium tetrahydroaluminate into trilithium hexahydroaluminate as a function of crystallite size obtained from XRPD line broadening.

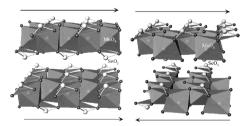
### Electronic behavior of three oxygen non-stoichiometric $Fe^{4+}/Fe^{3+}$ oxoperovskites

H.D. Zhou and J.B. Goodenough *Page 3679* 



Temperature dependences of (a) resistivity  $\rho(T)$  and  $d(\ln \rho)/d(1/T)$ ; (b) molar magnetic susceptibility  $\chi(T)$  and its inverse  $1/\chi(T)$ ; and (c) thermoelectric power  $\alpha(T)$  for Ca<sub>2</sub>Fe<sub>2</sub>O<sub>5,16</sub>. Inset of (c): Temperature dependences of magnetic susceptibility  $\chi(T)$  and thermoelectric power  $\alpha(T)$  for Ca<sub>2</sub>Fe<sub>2</sub>O<sub>5</sub>.

Synthesis and structural, spectroscopic and magnetic studies of two new polymorphs of Mn(SeO<sub>3</sub>) · H<sub>2</sub>O Aitor Larrañaga, José L. Mesa, José L. Pizarro, A. Peña, Roger Olazcuaga, María I. Arriortua and Teófilo Rojo *Page 3686* 

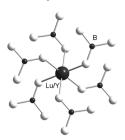


Crystal structures of two polymorphs of  $Mn(SeO_3) \cdot H_2O$ .

Continued

Luminescence properties of efficient X-ray phosphors of  $YBa_3B_9O_{18}$ ,  $LuBa_3(BO_3)_3$ ,  $\alpha$ - $YBa_3(BO_3)_3$  and  $LuBO_3$ 

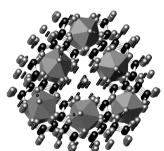
Chengjun Duan, Junlin Yuan and Jingtai Zhao Page 3698



Even though these compounds, YBa<sub>3</sub>B<sub>9</sub>O<sub>18</sub>, LuBa<sub>3</sub>(BO<sub>3</sub>)<sub>3</sub>,  $\alpha$ -YBa<sub>3</sub>(BO<sub>3</sub>)<sub>3</sub> and LuBO<sub>3</sub>, have different atomic structures, they have the common structural feature of each yttrium or lutetium ion bonded to six separate BO<sub>3</sub> groups, i.e., octahedral *RE*(BO<sub>3</sub>)<sub>6</sub> (*RE*=Lu or Y) moiety. This octahedral *RE*(BO<sub>3</sub>)<sub>6</sub>(*R*-*E*=Lu or Y) moiety seems to be an important structural element for efficient X-ray excited luminescence of those compounds, as are the edge-sharing octahedral TaO<sub>6</sub> chains for tantalate emission.

#### An open-framework three-dimensional indium oxalate: $[In(OH)(C_2O_4)(H_2O)]_3 \cdot H_2O$

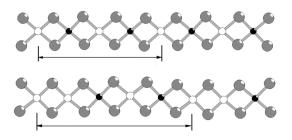
Sihai Yang, Guobao Li, Shujian Tian, Fuhui Liao and Jianhua Lin *Page 3703* 



An open-framework three-dimensional indium oxalate  $[In(OH)(C_2O_4)(H_2O)]_3 \cdot H_2O$  (1) was synthesized by hydrothermal reaction. Disordered water molecules are filled into the channels. It crystallizes in the trigonal system with space group R3c, a = 18.668(3) Å, c = 7.953(2) Å at 298 K.

### Synthesis, structure and properties of new chain cuprates, Na<sub>3</sub>Cu<sub>2</sub>O<sub>4</sub> and Na<sub>8</sub>Cu<sub>5</sub>O<sub>10</sub>

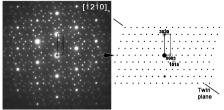
Mikhail Sofin, Eva-Maria Peters and Martin Jansen Page 3708



CuO2 chains in Na<sub>3</sub>Cu<sub>2</sub>O<sub>4</sub> (above) and Na<sub>8</sub>Cu<sub>5</sub>O<sub>10</sub> (below).

### Synthesis and structure investigation of the $Pb_3V(PO_4)_3$ eulytite

Roman V. Shpanchenko, Rodion V. Panin, Joke Hadermann, Catherine Bougerol, Eiji Takayama-Muromachi and Evgeny V. Antipov *Page 3715* 



The scheme at the left of the  $[\overline{1} \ 2 \ \overline{1} \ 0]_s^*$  pattern shows one of the two twins present in the  $[\overline{1} \ 2 \ \overline{1} \ 0]_s^*$  pattern and the indexation of this twin.

Synthesis, structural characterization, and solid-state NMR spectroscopy of  $[Ga(phen)(H_{1.5}PO_4)_2] \cdot H_2O$ and  $[Ga(phen)(HPO_4)(H_2PO_4)] \cdot 1.5H_2O$ (phen = 1, 10-phenanthroline), two organic-inorganic hybrid compounds with 1-D chain structures Wen-Jung Chang, Pai-Ching Chang, Hsien-Ming Kao and Kwang-Hwa Lii

Page 3722



Two hydrothermally synthesized organic–inorganic hybrid compounds consist of 1-D chains of strictly alternating GaO<sub>4</sub>N<sub>2</sub> octahedra and phosphate tetrahedra, which extend into 3-D supramolecular arrays via  $\pi$ - $\pi$  stacking interactions of *phen* ligands and hydrogen bonds. <sup>2</sup>H MAS NMR spectroscopy was applied to study the very short hydrogen bonds.

#### Syntheses and characterization of the samarium(III)– copper(II) 3D coordination network constructed by iminodiacetic acid

Yue-Peng Cai, Guo-Bi Li, Qing-Guang Zhan, Feng Sun, Jiang-Gao Zhang, Song Gao and An-Wu Xu *Page 3729* 

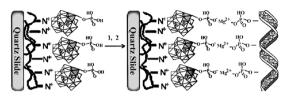


A reaction between  $Sm_2O_3$ , iminodiacetic acid (H<sub>2</sub>Idad), CuO, and H<sub>2</sub>O has allowed the synthesis of one nanoporous 3D open framework Cu(II)–Sm(III) coordination polymer, [{ $Sm_2Cu_3(I-dad)_6$ } · 8H<sub>2</sub>O]<sub>n</sub> (1) and then magnetic behavior of the compound, [{ $Gd_2Cu_3(Idad)_6$ } · 8H<sub>2</sub>O]<sub>n</sub> (2), with a similar structure was studied.

#### A novel biological active multilayer film based on polyoxometalate with pendant support-ligand

Huiyuan Ma, Jun Peng, Zhangang Han, Xia Yu and Baoxia Dong

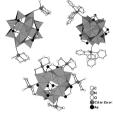
Page 3735



Key steps of immobilization of DNA to the {PDDA/ SiW\_11Co–PO\_4} film, 1 MgCl\_2 aqueous of 5 mM, 2 DNA aqueous.

### Hybrid inorganic–organic 1-D and 2-D frameworks with $\{As_8V_{14}O_{42}\}$ clusters as building blocks

Shou-Tian Zheng, Jie Zhang, Ji-Qing Xu and Guo-Yu Yang *Page 3740* 



Three inorganic–organic hybrid solid materials based on  $[As_8V_{14}O_{42}(H_2O)]^{4-}$  cluster building blocks bridging by transition metal complexes have been obtained by hydrothermal reaction and characterized by single-crystal X-ray diffraction. These compounds exhibit a wave-like chain, a tube-shaped chain and a rare two-dimensional structure containing interwinding puckery layers. Variable temperature susceptibility measurements demonstrate the presence of antiferromagnetic interaction between  $V^{\rm IV}$  cations in two one-dimensional structures.

3755

### Cumulative subject index