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CONTENTS

Editorial Announcement

Mercouri G. Kanatzidis Page 1295

Regular Articles

A novel ferrimagnetic irido-cuprate: IrSr₂GdCu₂O₈ A.J. Dos Santos-García, Myriam H. Aguirre, E. Morán, R. Saez Puche and M.Á. Alario-Franco *Page 1296*



IrSr₂GdCu₂O₈, prepared under high-temperature and highpressure conditions, is a new member of the M-1212-type cuprates. A ferrimagnetic Ir^{IV} -Gd^{III} spin ordering is observed below 15 K. The iridium oxidation state seems to be +4, while the copper oxidation state is Cu^{+2.5}.

Electron doping effect on structural and magnetic phase transitions in $Sr_{2-x}Nd_xFeMoO_6$ double perovskites

A.K. Azad, S.-G. Eriksson, Abdullah Khan, A. Eriksson and M. Tseggai *Page 1303*



3D ferrimagnetic structure of $Sr_{2-x}Nd_xFeMoO_6$ below Curie temperature.

Regular Articles—Continued

$$\label{eq:constraint} \begin{split} &[Zn_2(HPO_3)_2(H_2PO_3)][C_3H_5N_2] \text{ and } [Zn_2(HPO_3)_3] \\ &[C_4H_7N_2]_2 \cdot 2H_2O\text{: Two new layered zinc phosphites} \\ &\text{with double 12-membered rings templated by imidazole} \\ &\text{and 2-methylimidazole} \end{split}$$

Li Liu, Yunling Liu, Guanghua Li, Chao Chen, Minghui Bi and Wenqin Pang *Page 1312*



Polyhedral views of the double layer structures of $[Zn_2(HPO_3)_2(H_2PO_3)][C_3H_5N_2]$ and $[Zn_2(HPO_3)_3][C_4H_7N_2]_2 \cdot 2H_2O$ showing the imidazole cations sitting in the middle of the D12MR windows and 2-methylimidazole cations inserting into the D12MR cavities.

Synthesis, structure and properties of a new Zintl phase: SrLiSb

Shalabh Gupta and Ashok K. Ganguli *Page 1318*



An \sim [010] representation of the structure of SrLiSb. Indigo represent antimony atoms surrounded by red and the yellow spheres representing strontium and lithium atoms respectively forming the corners of trigonal prisms. The trigonal prisms are linked through Sr forming the zig-zag chains of trigonal prismatic columns. New representatives of the linear structure series containing empty Ga/Ge cubes in the Sm-Ga-Ge system Yaroslav O. Tokaychuk, Yaroslav E. Filinchuk, Anatoliy O. Fedorchuk, Artem Yu. Kozlov and Ivanna R. Mokra *Page 1323*



The structures of the new ternary compounds $\text{Sm}_2\text{Ga}_{7-x}\text{Ge}_x$ (x = 5.2-6.1) and $\text{Sm}_4\text{Ga}_{11-x}\text{Ge}_x$ (x = 5.76-8.75) belong to the linear intergrowth structure series built up from the segments of BaAl₄, AlB₂ and α -Po structure types. The Ga/ Ge networks in these structures contain characteristic empty cubes with one side capped by Ga atoms, which display an intrinsic displacive atomic disorder.

The effects of ZnGa₂O₄ formation on structural and optical properties of ZnO:Ga powders

Agnaldo de Souza Gonçalves,

Sergio Antonio Marques de Lima,

Marian Rosaly Davolos, Selma Gutierrez Antônio and Carlos de Oliveira Paiva-Santos *Page 1330*



Zoomed powder X-ray diffraction patterns of pure and gallium-doped zinc oxide samples.

Solid triphenylmethanol: A molecular material that undergoes multiple internal reorientational processes on different timescales

Simon J. Kitchin, Mingcan Xu, Heliodoro Serrano-González, Laura J. Coates, S. Zaka Ahmed, Christopher Glidewell and Kenneth D.M. Harris *Page 1335*



In solid triphenylmethanol, the molecules are arranged in hydrogen-bonded tetramers as shown; dynamic properties of this material are investigated here using solid-state ²H NMR spectroscopy.

Compatibility evaluation between La₂Mo₂O₉ fast oxide-ion conductor and Ni-based materials Gwenaël Corbel and Philippe Lacorre *Page 1339*



The absence of chemical reaction between Ni or NiO and $La_2Mo_2O_9$ up to 1000 °C, evidenced by room temperature X-ray powder diffraction, makes Ni-based cermet potential anode materials for LAMOX electrolyte.

Synthesis, structure, and characterization of a new one-dimensional tellurite phosphate, Ba₂TeO(PO₄)₂ Kang Min Ok and P. Shiv Halasyamani *Page 1345*



Ball-and-stick diagram showing one-dimensional structure of $Ba_2TeO(PO_4)_2$ in the *bc*-plane. Note the chains run along the *b*-axis.

Highly ordered MnO₂ nanowire array thin films on Ti/Si substrate as an electrode for electrochemical capacitor Cai-Ling Xu, Shu-Juan Bao, Ling-Bin Kong, Hua Li and Hu-Lin Li *Page 1351*



FESEM image of MnO_2 nanowire arrays grown on AAO/Ti/Si substance.

Continued

Luminescence of NaGdFPO₄: Ln^{3+} after VUV excitation: A comparison with GdPO₄: Ln^{3+} (Ln = Ce, Tb)

Zifeng Tian, Hongbin Liang, Huihong Lin, Qiang Su, Bei Guo, Guobin Zhang and Yibing Fu *Page 1356*



The VUV excitation (a, under emission at 312 nm) and VUVexcited emission (b, excitation under 155 nm) spectra for phosphor GdPO₄ at 293 K, the VUV excitation (c, under emission at 311 nm) and VUV-excited emission (d, excitation under 166 nm) spectra for phosphor NaGdFPO₄ at 293 K.

Single crystal structure and Raman spectrum of $Ba_3Na_2(CN_2)_4$





The crystal structure of $Ba_3Na_2(NCN)_4$ along the $\left[100\right]$ direction.

Combined powder neutron and X-ray diffraction study of charge and orbital order in Bi_{0.75}Sr_{0.25}MnO₃ R.J. Goff and J.P. Attfield *Page 1369*



A model for charge and orbital order in $Bi_{0.75}Sr_{0.25}MnO_3$ is proposed from a high-resolution powder X-ray and neutron diffraction study. An ordered intergrowth of antiferro-orbitally ordered (LaMnO₃ type) and charge and ferro-orbitally ordered (YBaMn₂O₆ type) blocks is found, in agreement with previous electron microscopy images.

Charge and structural ordering in the brownmillerite phases: $La_{1-x}Sr_xMnO_{2.5}$ (0.2 < x < 0.4)

Peter S. Casey, Daniel Barker and Michael A. Hayward Page 1375



Charge ordering in the octahedral layers of La_{0.75}Sr_{0.25}MnO_{2.5}.

Amorphous and nanocrystalline titanium nitride and carbonitride materials obtained by solution phase ammonolysis of Ti(NMe₂)₄

Andrew W. Jackson, Olga Shebanova, Andrew L. Hector and Paul F. McMillan *Page 1383*



Amorphous and nanocrystalline titanium nitrides and carbonitrides with a very defect-rich rocksalt structure.

Transport, magnetic, internal friction, and Young's modulus in the Y-doped manganites $La_{0.9-x}Y_{x}Te_{0.1}MnO_{3}$

G.H. Zheng, Y.P. Sun, X.B. Zhu and W.H. Song *Page 1394*



XRD patterns of the compound $La_{0.9-x}Y_xTe_{0.1}MnO_3$ (*x* = 0, 0.05, 0.10, 0.15).

Antiferromagnetic ordering with an anisotropy reversal in USn_{0.5}Sb_{1.5}

V.H. Tran, Z. Bukowski, J. Stępień-Damm and R. Troć *Page 1401*



(a) Temperature dependence of the reciprocal magnetic susceptibility of $USn_{0.5}Sb_{1.5}$ measured perpendicular (χ_{\perp}) and along (χ_{\parallel}) to the *c*-axis. (b) Magnetic susceptibility as a function of temperature.

Layer-by-layer assembly of multilayer films of polyoxometalates and tris(phenanthrolinedione) complexes of transition metals

Shuiying Gao, Xing Li, Chunpeng Yang, Taohai Li and Rong Cao

Page 1407



A series of organic–inorganic composite films $(BW_{12}/[M (phendione)_3]^{2+})_n (M = Fe^{2+}, Co^{2+})$ and $(Co_4(PW_9)_2/[M(phendione)_3]^{2+})_n (M = Fe^{2+}, Co^{2+})$, phendione = 1,10-phenanthroline 5,6-dione) were prepared by the layer-by-layer self-assembly method. The films exhibit well-defined electrochemical behaviors. Moreover, electrochemical behavior of the phendione species is pH dependent. The multilayer films have potential application in electrochemical sensors.

Synthesis, structure and optical limiting effect of a novel inorganic–organic hybrid polymer containing mixed chains of copper(I)/iodine

Hao-Hong Li, Zhi-Rong Chen, Jun-Qian Li, Hong-Bing Zhan, Wen-Xuan Zhang, Chang-Cang Huang, Cheng Ma and Bin Zhao *Page 1415*



An unusual coordination polymer $[(ebq)_2(Cu_3I_4)(CuI_2)]_n$ (1) has been synthesized and characterized. A highly interesting feature of 1 is its presence of mixed types of chains $[(Cu_3I_4)_n^-$ and $(CuI_2)_n^-$ chain] in one crystal lattice based on supramolecular self-assembly directed by cations. The infinite chains $(Cu_3I_4)_n^$ and $(CuI_2)_n^-$ in 1 could be described as the edge-sharing arrangement of CuI_4 tetrahedron. The optical limiting experiments show that the present polymer exhibits a large optical limiting capacity.

Template synthesis and characterization of PbTiO₃ nanowire arrays from aqueous solution M.C. Hsu, I.C. Leu, Y.M. Sun and M.H. Hon *Page 1421*



Side view image of $PbTiO_3$ nanowires bundle together after removing the AAO template.

Thermal decomposition of iron(VI) oxides, K_2FeO_4 and $BaFeO_4$, in an inert atmosphere

János Madarász, Radek Zbořil, Zoltán Homonnay, Virender K. Sharma and György Pokol *Page 1426*



Synthesis and characterization of $Sr_{0.75}Y_{0.25}Co_{1-x}M_xO_{2.625+\delta}$ (M=Ga, 0.125 $\leq x \leq 0.500$

and M = Fe, $0.125 \le x \le 0.875$) F. Lindberg, O.A. Drozhzhin, S.Ya. Istomin, G. Svensson, F.B. Kaynak, P. Svedlindh, P. Warnicke,

A. Wannberg, A. Mellergård and E.V. Antipov *Page 1434*



A possible arrangement of oxygen atoms in the oxygen-deficient layer of $Sr_{0.75}Y_{0.25}Co_{0.5}Fe_{0.5}O_{2.625+\delta}$ having crystal structure of perovskite related tetragonal phase $Sr_{0.75}Y_{0.25}CoO_{2.625}$ with unit cell parameters: $a=2a_{\rm p}$, and $c=4a_{\rm p}$ (314 phase).

Improvement of Er³⁺ emissions in oxyfluoride glass ceramic nano-composite by thermal treatment Daqin Chen, Yuansheng Wang, Yunlong Yu and En Ma

Page 1445



With increasing thermal treatment temperature, the emission intensities of ${}^{4}I_{13/2} \rightarrow {}^{4}I_{15/2}$, ${}^{4}F_{9/2} \rightarrow {}^{4}I_{15/2}$, and ${}^{2}H_{11/2}$, ${}^{4}S_{3/2} \rightarrow {}^{4}I_{15/2}$ transitions under 980 nm excitation are monotonously enhanced due to the incorporation of Er^{3+} into CaF_{2} nanocrystals homogeneously precipitated among glass matrix.

Structure-inheriting solid-state reactions under hydrothermal conditions

Kazuo Eda, Yuichi Uno, Noriko Nagai, Noriyuki Sotani, Chen Chen and M. Stanley Whittingham *Page 1453*



The present structure-inheriting solid-state reaction (SISSR) under a hydrothermal condition (ca. 10 bars and 453 K) enables us to markedly reduce the severe conditions for the usual synthesis of hp-CoMoO₄ via a solid-state phase transition (50 kbars and ca. 900 K).

Hydrothermal synthesis, crystal structure, thermal behavior, ferromagnetic resonance and ferrimagmetic behavior of $(C_4H_{12}N_2)_{1.5}[Fe_3(HAsO_4)_{1.02}(HPO_4)_{0.98}$ (AsO₄)_{0.88}(PO₄)_{0.12}F₅]

Begoña Bazán, José L. Mesa, José L. Pizarro, Luis Lezama, A. Peña, María I. Arriortua and Teófilo Rojo

Page 1459



Layered crystal structure of $(C_4H_{12}N_2)_{1.5}[Fe_3(HAsO_4)_{1.02}\ (HPO_4)_{0.98}(AsO_4)_{0.88}(PO_4)_{0.12}F_5].$

The defect chemistry of Ce(Pr, Zr)O_{2- δ}

D.P. Fagg, J.R. Frade, V.V. Kharton and I.P. Marozau *Page 1469*



Oxygen partial pressure dependence of total conductivity of $Ce_{0.8}Pr_{0.2}O_2$ at 950, 900, 850, 800 °C, in oxidising conditions (arrows indicate direction of increasing temperature), dashed and solid lines indicate fit to experimental data (points).

Hydrothermal synthesis and characterization of the first 1-D indiumphosphate chain $In_2(HPO_4)_2(H_2PO_4)_2F_2 \cdot C_4N_2H_{12}$, a precursor for

high dimensional structures

Chao Chen, Zhuo Yi, Minghui Bi, Yunling Liu, Chunyu Wang, Li Liu, Zan Zhao and Wenqin Pang *Page 1478*



A first 1-D indiumphosphate chain has been prepared by hydrothermal technique and the dimensional transformation was investigated, which proved the chain could be as a precursor to form high-dimensional complex open-framework.

Zirconium scandium oxide nitrides: Formation and decomposition followed in situ by XRD and thermal analysis

N.J. Martinez Meta and E. Schweda *Page 1486*



TG and DTA for the reoxidation of $Zr_{50}Sc_{12}O_{43}N_{50}$ to $Zr_{50}Sc_{12}O_{118}$ on air at a heating rate of 2 K.

A Raman spectroscopic study of the phase transition of $BaZr(PO_4)_2$: Evidence for a trigonal structure of the high-temperature polymorph

Thorsten Geisler, Karin Popa, Rudy J.M. Konings and Aurelian F. Popa

Page 1490



Raman mode frequencies of the PO_4 stretching vibrations in $BaZr(PO_4)_2$ as a function of temperature during heating and cooling across the phase transition temperature near 730 K.

A novel cobalt(II)-molybdenum(V) phosphate organic-inorganic hybrid polymer

Fa-Nian Shi, Filipe A. Almeida Paz, Penka I. Girginova, Helena I.S. Nogueira, João Rocha, Vítor S. Amaral, Jacek Klinowski and Tito Trindade *Page 1497*



A new organic–inorganic hybrid cobalt(II)–molybdenum(V) phosphate hybrid polymer, $(H_2pip)_3[Co_3Mo_{12}O_{24}(OH)_6 (PO_4)_8(H_{1.5}pip)_4] \cdot 5(H_2O)$ [where pip = piperazine], was isolated using hydrothermal synthesis, and characterised structurally by single-crystal X-ray diffraction, thermogravimetric analysis and vibrational spectroscopy. The magnetic properties of the material were also investigated.

Structure and physical properties of nonstoichiometric rare-earth cadmium antimonides, $RECd_{1-x}Sb_2$ (RE = La, Ce, Pr, Nd, Sm)

Andriy V. Tkachuk, Oksana Ya. Zelinska and Arthur Mar

Page 1506



 $\it RECd_{1-x}Sb_2$ adopts the HfCuSi_2-type structure, with layers of condensed $CdSb_4$ tetrahedra and Sb square nets.

A study of carboxylic-modified mesoporous silica in controlled delivery for drug famotidine

Qunli Tang, Yao Xu, Dong Wu and Yuhan Sun Page 1513



Famotidine dissolution curves and famotidine release profiles from the MS U-+ famo in the solution of simulated body fluid. Inset: correlation of the percent of released famotidine vs. the square root of leaching time $t^{1/2}$.

Electrochemical immobilization of Cs in single-crystalline SYNROC

Hideki Abe, Akira Satoh, Kenji Nishida, Eiji Abe, Takashi Naka, Motoharu Imai and Hideaki Kitazawa *Page 1521*



Optical microscope image of crystals grown at the tip of the working electrode.

The intercalation of cetyltrimethylammonium cations into muscovite by a two-step process: II. The intercalation of cetyltrimethylammonium cations into Li-muscovite Xiaofeng Yu, Liyan Zhao, Xiuxiang Gao, Xiaoping Zhang and Nianzu Wu Page 1525



The CTA⁺-intercalated muscovite composite with ordered structure has been obtained.

Two fluorescent coordination polymers constructed from mixed rigid and flexible carboxylate ligands: Formation of cross-linking helical and zigzag chains

Zhen Wang, Hanhui Zhang, Yiping Chen, Changcang Huang, Ruiqing Sun, Yanning Cao and Xiaohong Yu *Page 1536*

> helical chains down the c axis

View of structure of complex 2 down the *c*-axis, showing the cross-linking of helical chain units and zigzag chain units. Hydrogen atoms were removed for clarity.

Syntheses and crystal structures of three new borates templated by transition-metal complexes in situ

Guo-Ming Wang, Yan-Qiong Sun and Guo-Yu Yang Page 1545



Synthesis of maghemite sub-microspheres by simple solvothermal reduction method

Xian-Ming Liu, Shao-Yun Fu and Hong-Mei Xiao Page 1554



TEM photograph (a) and ED pattern (b) of the sample.

Hydrothermal synthesis and crystal structure of a new inorganic/organic hybrid of scandium sulfate: $(H_2en)Sc_2(SO_4)_4 \cdot (H_2O)_{0.72}$

Jianjiang Lu, John A. Schlueter and Urs Geiser *Page 1559*



The first organically templated layered structure of scandium sulfate, $(H_2en)Sc_2(SO_4)_4 \cdot (H_2O)_{0.72}$, (en = ethylenediamine) was synthesized by a hydrothermal method and characterized by single crystal X-ray diffraction. Thermogravimetric analysis indicates that this material is thermally stable to above 400 °C.

Preparation and electrorheological properties of triethanolamine-modified TiO_2

J.G. Cao, M. Shen and L.W. Zhou *Page 1565*



The yield stress and current of triethanolamine-modified ${\rm TiO}_2$ under DC electric field.

The intercalation of cetyltrimethylammonium cations into muscovite by a two-step process: I. The ion exchange of the interlayer cations in muscovite with Li⁺ Xiaofeng Yu, Liyan Zhao, Xiuxiang Gao, Xiaoping Zhang and Nianzu Wu Page 1569



Powder XRD diffraction patterns of original muscovite and muscovite after the first LiNO₃ treatment.

Bi_2Te_3 -Te nanocomposite formed by epitaxial growth of Bi_2Te_3 sheets on Te rod

Yuan Deng, Chang-Wei Cui, Ni-La Zhang, Tian-Hao Ji, Qing-Lin Yang and Lin Guo *Page 1575*



SEM image of an individual sheet-rod with EDX patterns (inset) taken from sheet and rod indicated by arrows.

Computational study of cation substitutions in apatites Toomas Tamm and Merike Peld Page 1581



Deformation of the hydroxide ion chain due to substitutions around the ion channel in substituted hydroxyapatites.

Crystal chemistry and crystallography of the SrR_2CuO_5 (*R* = lanthanides) phases

W. Wong-Ng, T. Haugan, J.A. Kaduk, R.A. Young, Z. Yang, M.H. Jang and M. Luong *Page 1588*



Seven-fold coordination of R in Sr R_2 CuO₅ (R = lanthanides) is shown inside a monocapped trigonal prism. Two such RO_7 units are joined to form the basic structure motif of R_2O_{11} .

Syntheses, structures, and magnetic properties of the europium(II) selenido pnictogenates(III), $EuPnSe_3$ (Pn = Sb, Bi)

Geng Bang Jin, Shane J. Crerar, Arthur Mar and Thomas E. Albrecht-Schmitt *Page 1596*



The isotypic compounds, EuPnSe₃ (Pn=Sb, Bi), have been prepared as pure phases via the reaction of Eu with Pn_2Se_3 (Pn=Sb, Bi) and Se. Their structures consist of square pyramidal $PnSe_5$ units and distorted $PnSe_6$ octahedra that form hollow columns that are separated by Eu²⁺ cations and Se₃²⁻ anions.

Effects of Al-doping on the stabilization of monoclinic \mbox{LiMnO}_2

Zu-Fei Huang, Chun-Zhong Wang, Xing Meng, Deng-Pan Wang and Gang Chen *Page 1602*



Total density of states (DOS) around $E_{\rm F}$ (0eV) without and with Al-doping for the (a) FM and (b) AF solutions. Spin-up/down states are plotted along the positive/negative ordinate.

NOTICE

The Keyword Index for Volume 179 will appear in the December 2006 issue as part of a cumulative index for the year 2006.