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### **Editorial Announcement**

Professor Wolfgang Tremel Mercouri G. Kanatzidis Page 1

### **Regular** Articles

### Crystal-structure and Mössbauer studies of

Li<sub>1.746</sub>Nd<sub>4.494</sub>FeO<sub>9.493</sub>

Miha Drofenik, Irena Ban, Darko Makovec, Darko Hanžel, Amalija Golobič and Ljubo Golič *Page 2* 



Representation of the  $Li_{1.746}Nd_{4.494}FeO_{9.493}$  structure.

# $Ag_3Ni_2O_4$ —A new stage-2 intercalation compound of 2H–AgNiO<sub>2</sub> and physical properties of 2H–AgNiO<sub>2</sub> above ambient temperature

Timo Sörgel and Martin Jansen *Page 8* 



 $\mathrm{Ag}_3\mathrm{Ni}_2\mathrm{O}_4\mathrm{--}$  the first stage-2 intercalation compound of a delafossite.

### **Regular** Articles—Continued

Synthesis, crystal structure and magnetic characterization of Na<sub>2</sub>Cu<sub>5</sub>(Si<sub>2</sub>O<sub>7</sub>)<sub>2</sub>: An inorganic ferrimagnetic chain António Moreira dos Santos, Paula Brandão,

Andrew Fitch, Mário S. Reis, Vítor S. Amaral and João Rocha *Page 16* 



A novel copper silicate was synthesized through hydrothermal methods. Its crystal structure was determined from powder diffraction data. It comprises zig-zag chains of copper dimers and trimers. Its magnetic behavior is characteristic of one dimensional ferrimagentism. A magnetic exchange sequence is proposed based on structural arguments.

Stabilization of hexagonal close-packed metallic nickel for alumina-supported systems prepared from Ni(II) glycinate

Vicente Rodríguez-González, Eric Marceau, Patricia Beaunier, Michel Che and Cyrille Train *Page 22* 



The decomposition of alumina-supported nickel glycinate in flowing argon mostly leads to an unusual phase of metallic Ni, hexagonal close-packed nanoparticles protected by graphite.

## The synthesis and structural characterization of the new ternary nitrides: $Ca_4TiN_4$ and $Ca_5NbN_5$

Janet L. Hunting, Marta M. Szymanski, Philip E. Johnson, C. Brenhin Kellar and Francis J. DiSalvo *Page 31* 



 ${\rm Ca}_4{\rm Ti}{\rm N}_4{\rm :}$  titanium tetrahedron (center) corner-sharing with calcium polyhedra.

## Structure and dielectric characterization of a new A-site deficient La<sub>5/3</sub>MgTaO<sub>6</sub> perovskite

D.D. Khalyavin, A.M.R. Senos, P.Q. Mantas,

D.N. Argyriou, I. Tarroso Gomes, L.G. Vieira and J.L. Ribeiro

### Page 41



Short-range vacancy ordering and octahedral tilting in  $La_{5/3}\ MgTaO_{6}.$ 

### Ionothermal synthesis of $\beta$ -NH<sub>4</sub>AlF<sub>4</sub> and the determination by single crystal X-ray diffraction of its room temperature and low temperature phases

Emily R. Parnham, Alex M.Z. Slawin and Russell E. Morris *Page 49* 



Ionothermal synthesis, the use of an ionic liquid as the solvent in materials preparation, has been used to prepare  $\beta$ -NH<sub>4</sub>AlF<sub>4</sub>, and structural characterisation indicates that there are two versions of the structure, a low temperature primitive phase at 93 K and a high temperature body-centered phase at 298 K.

### Local structure and oxidation state of uranium in some ternary oxides: X-ray absorption analysis

A.V. Soldatov, D. Lamoen, M.J. Konstantinović,S. Van den Berghe, A.C. Scheinost and M. Verwerft*Page 54* 



Comparison of the experimental U  $L_3$  edge XANES in BaUO<sub>3</sub> and NaUO<sub>3</sub> with the theoretical spectra.

Syntheses, crystal and electronic structure, and some optical and transport properties of LnCuOTe (Ln = La, Ce, Nd) Min Ling Liu, Li Bin Wu, Fu Qiang Huang, Li Dong Chen and James A. Ibers *Page 62* 



Crystal structure of LnCuOTe viewed approximately along [100].

**Product evolution in the Np(IV) fluorophosphate system** Travis H. Bray, Tyler A. Sullens, Tatiana Y. Shvareva, Richard E. Sykora, Richard G. Haire and Thomas E. Albrecht-Schmitt *Page 70* 



Two Np(IV) fluorophosphates, NpFPO<sub>4</sub> and  $Cs_2Np_2F_7PO_4$ , have been prepared as single crystals under hydrothermal conditions. NpFPO<sub>4</sub> crystallizes first, then reacts to yield  $Cs_2Np_2F_7PO_4$  and finally yields NpF<sub>4</sub>. Single crystal X-ray structures of NpFPO<sub>4</sub> and  $Cs_2Np_2F_7PO_4$  show three-dimensional frameworks containing Np(IV) in both eight- and nine-coordinate environments.

## Synthesis and properties of the double perovskites La<sub>2</sub>NiVO<sub>6</sub>, La<sub>2</sub>CoVO<sub>6</sub>, and La<sub>2</sub>CoTiO<sub>6</sub>

K.L. Holman, Q. Huang, T. Klimczuk, K. Trzebiatowski, J.W.G. Bos, E. Morosan, J.W. Lynn and R.J. Cava *Page 75* 



The antiferromagnetic structure of La<sub>2</sub>CoTiO<sub>6</sub> as prepared by high-temperature routes with spins showing the P2/m' magnetic symmetry.

### On $\alpha - \beta$ phase transition in cristobalite-type Al<sub>1-x</sub>Ga<sub>x</sub>PO<sub>4</sub> (0.00 $\leq x \leq 1.00$ )

S.N. Achary, R. Mishra, O.D. Jayakumar, S.K. Kulshreshtha and A.K. Tyagi *Page 84* 



The cristobalite-type GaPO<sub>4</sub> relaxed slowly to quartz type modification above 700  $^\circ C$  (as indicated by a broad exotherm in inset).

### Synthesis, structure and magnetic properties of R-W-O-N (R = Nd and Eu) oxynitrides

R. Pastrana-Fábregas, J. Isasi-Marín, C. Cascales and R. Sáez-Puche

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The scheelite-type structure of the new NdWO<sub>3.05</sub>N<sub>0.95</sub> oxynitride prepared by the nitridation of corresponding Nd<sub>2</sub>W<sub>2</sub>O<sub>9</sub> precursor. The magnetic susceptibility for this oxynitride has been successfully simulated using the semi-empirical structure derived CF parameters.

### Large-scale synthesis of single-crystal hexagonal tungsten trioxide nanowires and electrochemical lithium intercalation into the nanocrystals

Zhanjun Gu, Huiqiao Li, Tianyou Zhai, Wensheng Yang, Yongyao Xia, Ying Ma and Jiannian Yao *Page 98* 



The large-scale synthesis of single-crystal hexagonal tungsten oxides nanowires has been successfully realized by a simple hydrothermal method without any templates and catalysts. Uniform h-WO<sub>3</sub> nanowires with diameters of 25-50 nm and length of up to several micrometers are obtained. The electrochemical performances of the nanowires as anode materials of Li-ion batteries have also been investigated. These 1D nanostructures exhibit better cycle ability than that of bulk materials, which indicates the morphology and particle size have the influences on the electrochemical performances.

### The role of cation-cation interactions in a neptunyl chloride hydrate and topological aspects of neptunyl structural units T.Z. Forbes and P.C. Burns

**Page** 106



The structure of  $K_4(NpO_2)_3Cl_7(H_2O)_4$  contains neptunyl pentagonal bipyramids that are linked into chains through cation–cation interactions.

**Rb<sub>2</sub>BaNb<sub>2</sub>Se<sub>11</sub>: A new quaternary niobium polyselenide with infinite anionic chains composed of Nb<sub>2</sub>Se<sub>11</sub> building block Yuandong Wu, Christian Näther and Wolfgang Bensch** *Page 113* 



The  ${}_{\infty}^{1}$ [Nb<sub>2</sub>Se<sub>11</sub>]<sup>4-</sup> chain in the new mixed group1/group2 polyselenide compound Rb<sub>2</sub>BaNb<sub>2</sub>Se<sub>11</sub> is formed by interconnection of [Nb<sub>2</sub>Se<sub>11</sub>] units via Se<sub>2</sub><sup>2-</sup> dianions. The [Nb<sub>2</sub>Se<sub>11</sub>] building blocks are formed by face sharing of two distorted pentagonal bipyramidal NbSe<sub>7</sub> groups.

Hydrothermal synthesis of lindgrenite with a hollow and prickly sphere-like architecture Jiasheng Xu and Dongfeng Xue

Page 119



Lindgrenite  $[Cu_3(OH)_2(MoO_4)_2]$  with a hollow and prickly spherelike architecture has been synthesized via a hydrothermal route. The hierarchical lindgrenite particles are hollow and prickly spheres, which are comprised of numerous crystal strips that are aligned perpendicularly to the spherical surface.  $Cu_3Mo_2O_9$  with the similar size and morphology can be easily obtained by a thermal treatment of the as-prepared lindgrenite.

### Green and red upconversion luminescence in CeO<sub>2</sub>:Er<sup>3+</sup> powders produced by 785 nm laser Hai Guo

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Upconversion spectra of  $\text{Er}^{3+}$ -doped CeO<sub>2</sub> powders with different  $\text{Er}^{3+}$  concentration: (a) 0.5% (b) 1% (c) 3% (d) 6%, ( $\lambda_{ex} = 785 \text{ nm}$ ).

# Metal-organic frameworks from chiral square-pyramidal copper(II) complexes: Enantiospecific inclusion and perfectly polar alignment of guest and host molecules

Vamsee Krishna Muppidi, Panthapally S. Zacharias and Samudranil Pal

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The square-pyramidal Cu(II) complexes  $[CuL_2^n(H_2O)]$  with the bidentate  $HL^n$  ( $HL^1 = N$ -(2-hydroxy-5-nitrobenzyl)-(R)- $\alpha$ -methylbenzylamine and  $HL^2 = N$ -(2-hydroxy-5-nitrobenzyl)-(S)- $\alpha$ -methylbenzylamine) form 1:1 host–guest compounds with Br(CH<sub>2</sub>)<sub>2</sub>Br and CH<sub>3</sub>CN. The X-ray structures of these species reveal the enantiospecific confinement of the chiral rotamers of Br(CH<sub>2</sub>)<sub>2</sub>Br and perfectly polar ordering of both host and guest molecules in the crystal lattice. The figure shows the polar alignments of (a)  $[CuL_2^1(H_2O)] \cdot (P)$ -C<sub>2</sub>H<sub>4</sub>Br<sub>2</sub> and (b)  $[CuL_2^2(H_2O)] \cdot CH_3CN$ .

## EuBaFe<sub>2</sub>O<sub>5</sub>: Extent of charge ordering by Mössbauer spectroscopy and high-intensity high-resolution powder diffraction

P. Karen, K. Gustafsson and J. Lindén Page 138



Environments of the two crystallographically different Fe atoms in charge-ordered  $EuBaFe_2O_5$  at 100 K as refined from SXPD data; distances in Å.

## $EuBaFe_2O_{5+w}$ : Valence mixing and charge ordering are two separate cooperative phenomena

P. Karen, K. Gustafsson and J. Lindén





Effect of oxygen nonstoichiometry on valence mixing of di- and trivalent iron via electron sharing in ferromagnetically coupled pairs across the Eu layer in  $EuBaFe_2O_{5+w}$ .

## Chemical twinning of the pyrochlore structure in the system $Bi_2O_3$ -Fe\_2O\_3-Nb\_2O\_5

I.E. Grey, W.G. Mumme, T.A. Vanderah, R.S. Roth and C. Bougerol

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Polyhedral representation of the hexagonal  $Bi_{5.67}Nb_{10}FeO_{35}$  structure, viewed along [1 1 0]. Arrows show location of chemical twin planes. Bi atoms are shown as clusters of small circles. O' atoms (O(7), O(8) are shown as larger circles.

Continued

### Mild hydrothermal synthesis and magnetic properties of the manganates $Pr_{1-x}Ca_xMnO_3$

Yan Chen, Hongming Yuan, Ge Tian, Ganghua Zhang and Shouhua Feng *Page 167* 



The calcium-doped manganates,  $Pr_{1-x}Ca_xMnO_3$  (x = 0.39, 0.46, 0.70, 0.76), were synthesized as cube-shaped crystalline phases under mild hydrothermal conditions for the first time. The crystals could be grown in one step from solutions of metal salts and potassium hydroxide solution at temperatures ~240 °C. The studies indicate that formation of the materials is dependent on the alkalinity and composition of the initial reaction mixtures. The magnetic properties show spin-glass-like behavior due to competing ferromagnetic and antiferromagnetic exchange interactions in  $Pr_{1-x}Ca_xMnO_3$  with x = 0.39, 0.46.

Synthesis, structure and optical properties of new organic–inorganic haloplumbates complexes  $(C_5H_{10}N_3)PbX_4$  (X = Br, Cl),  $(C_2H_2N_4)PbBr_3$ Yinyan Li, Cuikun Lin, Guoli Zheng and Jun Lin *Page 173* 



Structure and optical properties of new layered organic–inorganic haloplumbate complexes, which combine haloplumbate and organic ammonium of histaminium and 3-amino-1,2,4-triazol were systematically studied.

### Formation of $\gamma$ -Fe<sub>2</sub>O<sub>3</sub> nanoparticles and vacancy ordering: An *in situ* X-ray powder diffraction study

Jens-Erik Jørgensen, Lene Mosegaard, Line E. Thomsen, Torben R. Jensen and Jonathan C. Hanson *Page 180* 



Stack of powder diagrams showing the formation of  $\gamma\text{-}Fe_2O_3$  nanoparticles and subsequent vacancy ordering at 305  $^\circ\text{C}.$ 

### Bridgman crystal growth of Yb<sub>2</sub>Ru<sub>3</sub>Ge<sub>4</sub>—A ternary germanide with a three-dimensional network of condensed distorted RuGe<sub>5</sub> and RuGe<sub>6</sub> units

Falko M. Schappacher, Kenichi Katoh and Rainer Pöttgen *Page 186* 



Condensation of the  $Ru1Ge_5$ ,  $Ru2Ge_6$ , and  $Ru3Ge_6$  units in the structure of  $Yb_2Ru_3Ge_4$ .

# The metal-rich palladium chalcogenides $Pd_2MCh_2$ (M = Fe, Co, Ni; Ch = Se, Te): Crystal structure and topology of the electron density

Regina Pocha, Catrin Löhnert and Dirk Johrendt Page 191



The metallic selenide Pd<sub>2</sub>CoSe<sub>2</sub> and homologue Pd<sub>2</sub>*MCh*<sub>2</sub> compounds (M=Fe, Co, Ni; Ch=Se, Te) are the first ternary palladium chalcogenides with iron group metals. The crystal structure shows one-dimensional  $\frac{1}{\infty}$ [CoSe<sub>4/2</sub>] tetrahedra with short Co–Co bonds, which are connected by Pd<sub>2</sub> dumbbells. Electronic structure calculations reveal strong metal–metal bonding.

V<sub>2</sub>Cu<sub>3</sub>Ga<sub>8</sub>, Mo<sub>2</sub>Cu<sub>3</sub>Ga<sub>8</sub> and W<sub>2</sub>Cu<sub>3</sub>Ga<sub>8</sub>—New compounds with a novel order variant of a bcc packing and motifs of selfsimilarity

Verena Kuntze, Rainer Lux and Harald Hillebrecht Page 198



Threefold capped cubes  $TMCu_3Ga_8$  are the coordination polyhedra in the new compounds  $TM_2Cu_3Ga_8$  (TM = V, Mo, W) which were synthesised from the elements. The new crystal structure can be described as an ordered defect variant of the bcc packing:  $[(TM)_2(Cu)_3(\Box)_3][Ga_8]$ . As a motif of self-similarity the polyhedra itself are packed in the same way.

## Synthesis, characterization, and fluorescent properties of two Pb(II) complexes: ${[Pb(hca)_2 \cdot DMF] \cdot DMF}_{\infty}$ and $[Pb(hca)_2(phen) \cdot DMF]_2$

Xu Qing-Feng, Zhou Qiu-Xuan, Lu Jian-Mei, Xia Xue-Wei and Zhang Yong *Page 207* 



Two novel Pb(II) complexes:  ${[Pb(hca)_2 \cdot DMF] \cdot DMF]_{\infty}}$  and  $[Pb(hca)_2(phen) \cdot DMF]_2$ , (hca = trans-4-hydroxycinnamic anion) were obtained and characterized. Their structures are also determined by X-ray crystal analysis. Both of complexes in DMF solution show visible fluorescence and the intensity is stronger than that of ligand. Their emission intensities are increased greatly in an alkaline solution of pH 8, which is due to the enhancement of the planar conjugation of ligand hca with the deprotonate of the phenolic group.

Direct growth of comet-like superstructures of Au–ZnO submicron rod arrays by solvothermal soft chemistry process Liming Shen, Ningzhong Bao, Kazumichi Yanagisawa, Yanqing Zheng, Kazunari Domen, Arunava Gupta and Craig A. Grimes *Page 213* 



One-step solvothermal synthesis of novel comet-like superstructures of radially standing ZnO submicron rod arrays.

 $Ni_{7-\delta}SnTe_2$ : Modulated crystal structure refinement, electronic structure and anisotropy of electroconductivity A.A. Isaeva, A.I. Baranov, Th. Doert, B.A. Popovkin, V.A. Kulbachinskii, P.V. Gurin, V.G. Kytin and V.I. Shtanov Page 221



Modulated crystal structure of  $Ni_{5.81} SnTe_2$  can be virtually generated from that of  $Ni_{2.76} Te_2.$ 

Low-temperature flux syntheses and characterizations of two 1-D anhydrous borophosphates: Na<sub>3</sub>B<sub>6</sub>PO<sub>13</sub> and Na<sub>3</sub>BP<sub>2</sub>O<sub>8</sub> Ding-Bang Xiong, Hao-Hong Chen, Xin-Xin Yang and Jing-Tai Zhao Page 233



Two new anhydrous sodium borophosphates Na<sub>3</sub>B<sub>6</sub>PO<sub>13</sub> and Na<sub>3</sub>BP<sub>2</sub>O<sub>8</sub> were synthesized by low-temperature molten salts techniques using boric acid and sodium dihydrogen phosphate as flux, respectively. Na<sub>3</sub>B<sub>6</sub>PO<sub>13</sub> crystallize in *Pnma* and comprise infinite chain of  $\frac{1}{\infty}$ {[B<sub>6</sub>PO<sub>13</sub>]<sup>3-</sup>, and Na<sub>3</sub>BP<sub>2</sub>O<sub>8</sub> crystallize in *C*2/*c* and comprise infinite chain of  $\frac{1}{\infty}$ {[BP<sub>2</sub>O<sub>8</sub>]<sup>3-</sup>.

## Third- and second-order optical nonlinearity of Ge-Ga-S-PbI<sub>2</sub> chalcohalide glasses

Haitao Guo, Haizheng Tao, Shaoxuan Gu, Xiaolin Zheng, Yanbo Zhai, Saisai Chu, Xiujian Zhao, Shufeng Wang and Qihuang Gong

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Second-harmonic generation (SHG) has been observed from thermally poled Ge–Ga–S–PbI<sub>2</sub> glasses by utilizing Maker fringe method. Ultrafast third-order nonlinear optical responses of these glasses have been measured by using femtosecond time-resolved optical Kerr effect (OKE) technique at the wavelength of 820 nm.

#### New misfit-layered cobalt oxide (CaOH)<sub>1.14</sub>CoO<sub>2</sub>

Mitsuyuki Shizuya, Masaaki Isobe, Yuji Baba, Takuro Nagai, Minoru Osada, Kosuke Kosuda, Satoshi Takenouchi, Yoshio Matsui and Eiji Takayama-Muromachi *Page 249* 



Crystal-structure model of the misfit-layered cobalt oxide  $(CaOH)_{1.14}CoO_2$ . The rectangles indicate unit cells of the two subsystems. The open circles and squares represent the cobalt atoms situated at different positions along the projected coordinate.

#### Continued

## An organically templated yttrium fluoride with a 'Super-Diamond' structure

Nicholas F. Stephens and Philip Lightfoot *Page 260* 



The organically templated yttrium fluoride  $[C_3N_2H_{12}]_{0.5}[Y_3F_{10}]$  adopts a 'Super-Diamond' framework structure. Its hydrothermal synthesis and structure determination from powder X-ray diffraction (PXRD) are described.

Structural characterization, thermal and electric properties of imidazolium bromoantimonate(III): [C3H<sub>5</sub>N<sub>2</sub>]<sub>3</sub>[Sb<sub>2</sub>Br<sub>9</sub>] A. Piecha, V. Kinzhybalo, K. Ślepokura and R. Jakubas *Page 265* 



Projection of the crystal structure of  $[C_3H_5N_2]_3[Sb_2Br_9]$  at 100 K (form I) on the cb plane as a polyhedral representation.

## Nanosized aluminum nitride hollow spheres formed through a self-templating solid-gas interface reaction

Jie Zheng, Xubo Song, Yaohua Zhang, Yan Li, Xingguo Li and Yikang Pu

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Nanosized aluminum nitride hollow spheres were synthesized by nitridation of aluminum nanoparticles at  $1000\,^\circ\mathrm{C}$  using ammonia.

### Microemulsion-mediated hydrothermal synthesis and characterization of zircon-type LaVO<sub>4</sub> nanowires Weiliu Fan, Xinyu Song, Sixiu Sun and Xian Zhao

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The zircon-type tetragonal (*t*-) LaVO<sub>4</sub> nanowires were controlled synthesized by a microemulsion-mediated hydrothermal method, in which the aqueous cores of SDS/cyclohexane/*n*-hexanol/water microemulsion were used as constrained microreactors for a controlled growth of *t*-LaVO<sub>4</sub> nanocrystals under hydrothermal conditions.

Nanoparticles of superconducting  $\gamma$ -Mo<sub>2</sub>N and  $\delta$ -MoN A. Gomathi, A. Sundaresan and C.N.R. Rao *Page 291* 



TEM image of the  $\gamma$ -Mo<sub>2</sub>N particles with the inset showing the resistivity of the sample as a function of temperature.

Cation distribution and magnetic properties in chromiumsubstituted nickel ferrites prepared using aerosol route Sonal Singhal and Kailash Chandra

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Hysterisis loop of chromium-substituted nickel ferrites after annealing at 1200  $^\circ \! \mathrm{C}.$ 

## Fabrication and characterization of cerium-doped barium titanate inverse opal by sol-gel method

Yi Jin, Yihua Zhu, Xiaoling Yang, Chunzhong Li and Jinghong Zhou

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Cerium-doped barium titanate inverted opal was synthesized from barium acetate acid contained cerous acetate and tetrabutyl titanate in the interstitial spaces of a PS opal, which involves infiltration of precursors into the interstices of the PS opal template and removal of the PS opal by calcination.

## Synthesis and structure determination of $Co(HNCN)_2$ and $Ni(HNCN)_2$

Manuel Krott, Xiaohui Liu, Paul Müller and Richard Dronskowski

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Crystal structure of  $Co(HNCN)_2$  and  $Ni(HNCN)_2$  with Co/Ni atoms as white, N as grey, C as dark-grey, and H as light-grey balls.

Structure and electron density analysis of electrochemically and chemically delithiated LiCoO<sub>2</sub> single crystals Yasuhiko Takahashi, Norihito Kijima, Kaoru Dokko, Matsuhiko Nishizawa, Isamu Uchida and Junji Akimoto Page 313



Three-dimensional electron density distribution of the electrochemically delithiated  $\rm Li_{0.68}CoO_2$  obtained by the maximum entropy method (MEM) using single-crystal X-ray diffraction data.

Structural characterization of the hollandite host lattice for the confinement of radioactive cesium: Quantification of the amorphous phase taking into account the incommensurate modulated character of the crystallized part

A.Y. Leinekugel-le-Cocq-Errien, P. Deniard, S. Jobic, E. Gautier, M. Evain, V. Aubin and F. Bart *Page 322* 



Unusual one-dimensional branched-chain structures assembled by a novel imidazole-containing tripodal ligand with cadmium(II) salts and their fluorescent property Ling-Yan Kong, Xi-Hong Lu, Yong-Qing Huang, Hiroyuki Kawaguchi, Qian Chu, Hui-Fang Zhu and Wei-Yin Sun

Page 331



Three novel coordination polymers  $[Cd_3(L)_2(\mu-Br)(\mu-Cl)Br_3Cl]$  (1),  $[Cd_3(L)_2(\mu-Cl)_2Cl_4]$  (2) and  $[Cd(L)Cl]_2[CdCl_4] \cdot H_2O$  (3) with onedimensional branched chain and zigzag chain structures were obtained by reactions of an imidazole-containing tripodal ligand  $N^1$ -(2-aminoethyl)- $N^1$ -(2-imidazolethyl)-ethane-1,2-diamine (L) with Cd(II) salts.

## Mössbauer spectra as a "fingerprint" in tin-lithium compounds: Applications to Li-ion batteries

F. Robert, P.E. Lippens, J. Olivier-Fourcade, J.-C. Jumas, F. Gillot, M. Morcrette and J.-M. Tarascon *Paae 339* 



 $\Delta - \delta$  correlation diagram for the different tin sites of the Li–Sn compounds. The symbols denote the different Li–Sn phases and the products obtained at the end of the discharge of  $\eta$ -Cu<sub>6</sub>Sn<sub>5</sub> and SnB<sub>0.6</sub>P<sub>0.4</sub>O<sub>2.9</sub>. The grey and the light-grey areas show Sn-centred polyhedra without and with one Sn first-nearest neighbours, respectively.

#### Continued

*Ln*SrScO4 (Ln = La, Ce, Pr, Nd and Sm) systems and structure correlations for  $A_2BO_4$  ( $K_2NiF_4$ ) structure types Rina Patel, Charles Simon and Mark T. Weller *Page 349* 



Tilting of the octahedra in  $K_2NiF_4$  structure type oxides ( $A_2BO_4$ ) may be controlled by the *A*-type cation size and by temperature.

## Structural evolution of $(Ca_{0.35}Sr_{0.65})TiO_3$ perovskite at high pressures

Michael A. Carpenter, Susana Rios, Peter Sondergeld, Wilson Crichton and Pierre Bouvier

### Page 360



Variation of the tetragonal strain,  $e_{tz}$ , as a function of pressure for Ca<sub>0.35</sub>Sr<sub>0.65</sub>TiO<sub>3</sub>, showing a break in slope in the vicinity of 3–4 GPa.

Three-layer Aurivillius phases containing magnetic transition metal cations:  $Bi_{2-x}Sr_{2+x}(Nb,Ta)_{2+x}M_{1-x}O_{12}$ ,  $M = Ru^{4+}$ ,  $Ir^{4+}$ ,  $Mn^{4+}$ ,  $x \approx 0.5$ 

Neeraj Sharma, Chris D. Ling, Grant E. Wrighter, Parry Y. Chen, Brendan J. Kennedy and Peter L. Lee *Page 370* 



Structure of Bi1.5Sr2.5Nb2.5Ru0.5O12.

### Neutron diffraction and X-ray absorption study of Ag<sub>5</sub>Pb<sub>2</sub>O<sub>6</sub>

K. Yoshii, M. Mizumaki, K. Kato, T. Uruga, H. Abe, A. Nakamura, Y. Shimojo, Y. Ishii and Y. Morii *Page 377* 



Powder neutron diffraction patterns of  $Ag_5Pb_2O_6$  at room temperature.

### **Rapid Communication**

Two unprecedented inorganic-organic boxlike and chainlike hybrids based on arsenic-vanadium clusters linked by nickel complexes

Yanfei Qi, Yangguang Li, Enbo Wang, Hua Jin, Zhiming Zhang, Xinglong Wang and Song Chang *Page 382* 



The boxlike structure of compound **1** with cavity is designed from  $[{Ni(en)_2}_4(4,4'-bipy)_4{Ni(H_2O)_2}]$  sheets pillared by  $[\alpha-As_8V_{14}O_{42}]$  clusters, which represents the first mixed-organic ligand-decorated tetrameric As–V–O cluster.

## Comment on "Preparation and electrorheological properties of triethanolamine-modified TiO<sub>2</sub>"

F.F. Fang and H.J. Choi *Page 390* 



Universal yield stress plot of  $\hat{\hat{\tau}}$  versus  $\hat{E}$  for triethanolaminemodified TiO<sub>2</sub> based on ER fluid various electric fields.

Synthesis, structure and photochromic properties of a novel 1,6-hexanediamine trimolybdate supramolecular compound Dehui Sun, Hongjie Zhang, Jilin Zhang, Guoli Zheng, Jiangbo Yu and Shuyan Gao *Page 393* 



Crystal structure of 1,6-hexanediamine trimolybdate  $(C_6H_{18}N_2)[Mo_3O_{10}]$  along *c*-axis. It consists of protonated 1,6-hexanediamine (HDA) and novel infinite chains  $[Mo_3O_{10}]^{2-}$ . Infinite chains  $[Mo_3O_{10}]^{2-}$  are made up of distorted  $MoO_6$  octahedron connected by edges and corners and are linked through protonated HDA cations into a one-dimensional network. What is more, the compound displays photochromic properties and may be applied to the field of photosensitive materials.

### Author inquiries

### Submissions

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