JOURNAL OF SOLID STATE CHEMISTRY

Volume 179, Number 8, August 2006

CONTENTS

Foreword

Professor Hans Georg von Schnering celebrates his 75th birthday Reinhard Nesper and Yuri Grin Page 2251

Special Section: Dedicated to the occasion of the 75th birthday of Prof. Hans Georg von Schnering

 $\begin{array}{l} Thermoelectric \ properties \ and \ microstructure \ of \ Mg_3Sb_2\\ Cathie \ L. \ Condron, \ Susan \ M. \ Kauzlarich, \ Franck \end{array}$

Gascoin and G. Jeffrey Snyder *Page 2252*



Dimensionless figure of merit for Mg_3Sb_2 hot pressed and sintered at 873 K. The inset illustrates the crystal structure of Mg_3Sb_2 along the [100] direction (white = Mg, black = Sb).

The lanthanoid(III) chloride *cyclo*-tetrasilicates $M_6Cl_{10}[Si_4O_{12}]$ (M=Sm, Gd–Dy): Synthesis, structure and IR investigations

Ingo Hartenbach, Stefan Jagiella and Thomas Schleid Page 2258



Cyclo-oxotetrasilicate unit in M_6 Cl₁₀[Si₄O₁₂].

A density-functional and molecular-dynamics study on the physical properties of yttrium-doped tantalum oxynitride

H. Wolff, H. Schilling, M. Lerch and R. Dronskowski *Page 2265*



Structural result of a room-temperature molecular-dynamic simulation of a supercell of $Y_{0.125}Ta_{0.875}O_{0.875}N \square_{0.125}$.

Fabrication of MnAs microstructures on GaAs(001) substrates and their electrical properties

Y. Takagaki, E. Wiebicke, L. Däweritz and K.H. Ploog



Surface of a partly etched MnAs film grown on a GaAs(001) substrate.

Thermal stability of high surface area silicon carbide materials

Piotr Krawiec and Stefan Kaskel Page 2281



The synthesis of mesoporous silicon carbide by chemical vapor infiltration of dimethyl dichlorosilane into mesoporous silica SBA-15 and subsequent dissolution of the silica matrix was used for the preparation of mesoporous SiC with high specific surface areas up to $830 \text{ m}^2 \text{g}^{-1}$ and pore sizes between 2 and 10 nm.

On the distribution of tetrelide atoms (Si, Ge) in $Gd_5(Si_xGe_{1-x})_4$

Sumohan Misra and Gordon J. Miller *Page 2290*



The Ge occupation in each T site in $Gd_5(Si_xGe_{1-x})_4$ is studied as a function of Si concentration, x. The different crystal structures are related to the fractions of Ge–Ge (solid), Si–Ge (dashed) and Si–Si (solid) dimers at the T1–T1 sites.

M_{1-x} [W₂O₂X₆] with $M = K^+$, Tl⁺, Ag⁺, Hg²⁺, Pb²⁺; X =Cl, Br—A class of mixed valence tungsten (IV,V) compounds with layered structures, W–W bonds and high conductivity

Johannes Beck, Christian Kusterer, Rolf-Dieter Hoffmann and Rainer Pöttgen *Page 2298*



 WOCl_3 has a particular reactivity to form non-stoichiometric quaternary compounds $M_{1-x}[W_2O_2Cl_6]$ with mono and divalent cations. The compounds exhibit temperature independent paramagnetism and high electrical conductivity.

Mn_5Si_3 -type host-interstitial boron rare-earth metal silicide compounds RE_5Si_3 : Crystal structures, physical properties and theoretical considerations

Jérome Roger, Mouna Ben Yahia, Volodymyr Babizhetskyy, Joseph Bauer, Stéphane Cordier, Roland Guérin, Kurt Hiebl, Xavier Rocquefelte, Jean-Yves Saillard and Jean-François Halet *Page 2310*



Incorporation of boron in vacant octahedral sites of the $Mn_5Si_3\mbox{-type}$ phase Gd_5Si_3 modifies its resistivity properties.

Barrelane-like germanium clusters in Eu₃Ge₅: Crystal structure, chemical bonding and physical properties Sergij Budnyk, Franz Weitzer, Christof Kubata, Yurii Prots, Lev G. Akselrud, Walter Schnelle, Kurt Hiebl, Reinhard Nesper, Frank R. Wagner and Yuri Grin Page 2329



Main building blocks of the crystal structure Eu_3Ge_5 are $[Ge_5]^{6-}$ cluster anions surrounded by Eu^{2+} cations. The nearly tetragonal-pyramidal shape is suggested by the interatomic distances. Contrary to that, the bonding analysis with the ELF reveals only two- and three-bonded germanium atoms forming a strongly distorted [111]-barrelane-like cluster.

Synthesis and characterisation of hexagonal molybdenum nitrides

Alexey Yu. Ganin, Lorenz Kienle and Grigori V. Vajenine





Hexagonal δ_2 -MoN with the NiAs-type crystal structure.

Regular Articles

Chemical shifts of atomic core levels and structure of $K_{1-x}Ti_{1-x}Sb_xOPO_4$, x=0-0.23, solid solutions V.V. Atuchin, O.A. Alekseeva, V.G. Kesler, L.D. Pokrovsky, N.I. Sorokina and V.I. Voronkova *Page 2349*



Dependence of $\varDelta({\rm O}$ 1s–Ti 2 $p_{3/2})$ on $L({\rm Ti–O})$ for KTP family crystals.

A novel blue-emitting phosphor LiSrPO₄:Eu²⁺ for white LEDs





The EL spectrum of the blue LED-based $LiSrPO_4:Eu^{2+}$.

PbI₄Cu₂(PPh₃)₄: A heterometallic iodide with unusual *cis*-divacant octahedral coordination sphere for lead: Synthesis, structure, red-infrared fluorescence and theoretical studies

Le-Qing Fan, Yi-Zhi Huang, Li-Ming Wu, Ling Chen, Jun-Qian Li and En Ma *Page 2361*



A new heterometallic iodide, PbI₄Cu₂(PPh₃)₄, was synthesized by reactions of PbI₂, CuI and triphenylphosphine (PPh₃) in DMF solution. The single-crystal X-ray diffraction analyses show that Pb(II) center adopts an unusual *cis*-divacant octahedral geometry. DFT calculations and fragment orbital interaction analyses reveal the presence of a 3c-4e hypervalent bonding about lead and the formation of the unusual *cis*divacant [PbI₄]²⁻ octahedron is energetically favorable. The title yellow compound has an optical bandgap of 2.69 eV and shows remarkable red-infrared fluorescence emission.

Regular Articles—Continued

Self-assembly of four new extended architectures based on reduced polyoxometalate clusters and cadmium complexes

Ying Ma, Yangguang Li, Enbo Wang, Ying Lu, Xinlong Wang and Xinxin Xu *Page 2367*



In this paper, we report four new extended architectures based on reduced polyoxometalate clusters and cadmium complexes. Compounds 1–4 are built of $Cd[P_4Mo_6]_2$ dimers as the basic structural motif and Cd–4,4'-bpy, Cd–phen and Cd–2,2'-bpy complexes as the linkers to constructed novel 2D layer structure.

Structural, magnetic, and spectroscopic studies of YAgSn, TmAgSn, and LuAgSn

C. Peter Sebastian, Hellmut Eckert, Constanze Fehse, Jon P. Wright, J. Paul Attfield, Dirk Johrendt, Sudhindra Rayaprol, Rolf-Dieter Hoffmann and Rainer Pöttgen

Page 2376



Crystal Structure of YAgSn.

Anion mediated polytype selectivity among the basic salts of Co(II)

T.N. Ramesh, Michael Rajamathi and P. Vishnu Kamath



(a) Observed PXRD pattern of cobalt hydroxytartarate compared with the DIFFaX simulated patterns of (b) $3R_1$ and (c) $3R_2$ polytypes, respectively.

A crystallographic description of experimentally identified formation reactions of Cu(In,Ga)Se₂ F. Hergert, S. Jost, R. Hock and M. Purwins *Page 2394*



The epitaxial connection of the crystal structures of β -Cu₂Se (bottom) and β -In₂Se₃ (top) is the initiating step of one possible solid-state reaction for the formation of α -CuInSe₂.

A new anatase-type phase in the system Mg-Ta-O-N

H. Schilling, M. Lerch, A. Börger, K.-D. Becker, H. Wolff, R. Dronskowski, T. Bredow, M. Tovar and C. Baehtz

Page 2416



Schematic representation (constant 30 valencies) of all new compounds obtained as single phase samples in the system Mg-Ta-O-N (dark gray symbols).

Synthesis, structure and magnetic properties of porous magnetic composite, based on MCM-41 molecular sieve with Fe_3O_4 nanoparticles

Sergey V. Kolotilov, Oleksiy Shvets, Olivier Cador, Natalia Kasian, Vyacheslav G. Pavlov, Lahcène Ouahab, Vladimir G. Ilyin and Vitaly V. Pavlishchuk *Page 2426*



Schematic presentation of MCM-41/Fe₃O₄ composite.

A novel Mo(V) oligophosphate built up of di- and triphosphate groups: Cs(MoO)₄(P₂O₇)₂(P₃O₁₀) André Leclaire and Bernard Raveau *Page 2433*



The structure of Cs(MoO)₄(P_2O_7)₂(P_3O_{10}) viewed along **a** with one P_3O_{10} group and one MoP₂O₁₁ unit headlined.

First-principles relativistic calculation for 4*f*-5*d* **transition energy of** Ce³⁺ **in various fluoride hosts** Shinta Watanabe, Takugo Ishii, Koji Fujimura and Kazuyoshi Ogasawara

Page 2438



Correlation diagram between the experimental 1st peak energy and the theoretical 1st peak energy. The left figure (A) shows the results without the lattice relaxation by correction of bond length and right one (B) shows the results with the lattice relaxation by correction of bond length. The corresponding coefficients of correlation R are 0.78 and 0.98, respectively.

Phase coexistence in $CaCu_xMn_{7-x}O_{12}$ solid solutions W. Sławiński, R. Przeniosło, I. Sosnowska,

M. Bieringer, I. Margiolaki, A.N. Fitch and E. Suard *Page 2443*



Schematic representation of the trigonal $CaCu_xMn_{7-x}O_{12}$ unit cell shown in the rhombohedral setting of space group $R\overline{3}$.

A one-step solvothermal route for the synthesis of nanocrystalline anatase TiO₂ doped with lanthanide ions Daniele Falcomer, Matteo Daldosso, Carla Cannas, Anna Musinu, Barbara Lasio, Stefano Enzo, Adolfo Speghini and Marco Bettinelli





HRTEM image of Eu³⁺ doped anatase TiO₂ nanocrystalline powders prepared by a solvothermal technique.

Selective substitution of vanadium for molybdenum in $Sr_2(Fe_{1-x}V_x)MoO_6$ double perovskites

Q. Zhang, G.H. Rao, Q. Huang, X.M. Feng, Z.W. Ouyang, G.Y. Liu, B.H. Toby and J.K. Liang Page 2458



Magnetic structure models with the moments aligning along [110], [100] and [111] directions, respectively, for $Sr_2(Fe_{1-x}V_x)$ MoO₆ compounds.

Synthesis, crystal structure and charge distribution of Na₇As₁₁O₃₁: An oxygen-deficient layered sodium arsenate

Abderrahmen Guesmi, Massimo Nespolo and Ahmed Driss

Page 2466



Perspective view of the layer structure of the oxygen-deficient sodium arsenate Na₇As₁₁O₃₁.

Preparation, crystal structure and chemical bonding analysis of the new binary compounds Rh₄Ga₂₁ and Rh₃Ga₁₆

Magnus Boström, Yurii Prots and Yuri Grin Page 2472



Crystal structures of Rh₄Ga₂₁ and Rh₃Ga₁₆.

The mercury chromates Hg₆Cr₂O₉ and Hg₆Cr₂O₁₀-Preparation and crystal structures, and thermal behaviour of Hg₆Cr₂O₉ Matthias Weil and Berthold Stöger Page 2479



Hg₆Cr₂O₉ (left) and Hg₆Cr₂O₁₀ (right): details of the Hg–O network.

Synthesis, structures and phase transitions in the double perovskites Sr_{2-r}Ca_rCrNbO₆

Melina C.L. Cheah, Brendan J. Kennedy, Ray L. Withers, Masao Yonemura and Takashi Kamiyama Page 2487



Variation of the lattice parameters and volume in the series $Sr_{2-x}Ca_xCrNbO_6$. The lattice parameters in the monoclinic phase have been scaled for ease of comparison. The solid line is a linear fit to variation in volume.

Local crystal chemistry, structured diffuse scattering and the dielectric properties of $(Bi_{1-x}Y_x)_2(M^{III}Nb^V)O_7$ $(M=Fe^{3+}, In^{3+})$ Bi-pyrochlores

W. Somphon, V. Ting, Y. Liu, R.L. Withers, Q. Zhou and B.J. Kennedy

Page 2495



The pattern of correlated O'Bi₄ tetrahedral rotation around the $\langle 111 \rangle$ axis responsible for the observed $\langle 111 \rangle^*$ rods of diffuse intensity in Bi-pyrochlores.

Preparation, structural study from neutron diffraction data and magnetism of the disordered perovskite $Ca(Cr_{0.5}Mo_{0.5})O_3$

M.J. Martínez-Lope, J.A. Alonso, M.T. Casais, M. García-Hernández and V. Pomjakushin *Page 2506*



Ca(Cr_{0.5}Mo_{0.5})O₃ is orthorhombic, *Pbnm* space group, and exhibits a complete disordering of Cr³⁺ and Mo⁵⁺ over the *B*-site of the perovskite. The magnetic susceptibility is characteristic of a ferrimagnetic behavior, with $T_{\rm C}$ =125 K, and a small saturation magnetization at T=5 K, of 0.05 $\mu_{\rm B}$ /f.u.

Properties of cerium-zirconium mixed oxides partially substituted by neodymium: Comparison with Zr-Ce-Pr-O ternary oxides

Jana Mikulova, Sylvie Rossignol, Francois Gérard, Danielle Mesnard, Charles Kappenstein and Daniel Duprez *Page 2511*



Variation of oxygen vacancies under hydrogen on ternary oxides.

Unusual supramolecular assembly and nonlinear optical properties of L-histidinium hydrogen malate

E. de Matos Gomes, V.H. Rodrigues, M.M.R. Costa, M.S. Belsley, P.J.M. Cardoso, C.F. Gonçalves and F. Proença

Page 2521



One-dimensional malate chains running along [100]. The anions form head-to-side chains where the COO^- group of one anion is hydrogen bonded to the COH side group of a neighbor one.

Controlled peak wavelength shift of

 $Ca_{1-x}Sr_x(S_ySe_{1-y}):Eu^{2+}$ phosphor for LED application Mihail Nazarov and Chulsoo Yoon Page 2529



Peak wavelength diagram for $(Ca_{1-x}Sr_x)(S_{1-y}Se_y):Eu^{2+}$.

A series of borate-rich metalloborophosphates $Na_2[M^{II}B_3P_2O_{11}(OH)] \cdot 0.67H_2O$ ($M^{II} = Mg$, Mn, Fe, Co, Ni, Cu, Zn): Synthesis, structure and magnetic susceptibility

Tao Yang, Guobao Li, Jing Ju, Fuhui Liao, Ming Xiong and Jianhua Lin



A series of metalloborophosphates $Na_2[M^{II}B_3P_2O_{11}(OH)] \cdot 0.67H_2O (M^{II} = Mg, Mn, Fe, Co, Ni, Cu, Zn)$ were synthesized under hydrothermal conditions (473 K). The structure consists of microporous 3D open framework with 12-membered ring channels composed of octahedral ($M^{II}O_6$), tetrahedral (BO₄, PO₄) and triangular (BO₂(OH)) units.

Hydrothermal synthesis and structure of a novel 3D framework based on ξ -octamolybdate chains: [Cu₂(quinoxaline)₂Mo₄O₁₃]_n

Li-Juan Chen, Can-Zhong Lu, Xiang He,

Quan-Zheng Zhang, Wen-Bin Yang and Xin-hua Lin Page 2541



A novel three-dimensional framework constructed from ξ -octamolybdate chains integrated by pairs of 1D copperquinoxaline polymer chains.

Preparation and formation mechanism of wood-block-like calcite particles

Hua Guo, Jiaguo Yu and Bei Cheng Page 2547



Pure calcite crystal with different morphologies such as woodblock and spherical aggregates were prepared by a simple precipitation reaction in the presence of citric acid and the formation mechanism was proposed.

Electrochemical reaction of lithium with nanosized vanadium antimonate

Julián Morales, Luis Sánchez, Francisco Martín and Frank Berry *Page 2554*

VSbO4 50 nm —

TEM image of nanosized VSbO₄ sample.

Fabrication and photoelectrochemical properties of porous ZnWO₄ film

Xu Zhao, Wenqing Yao, Yan Wu, Shicheng Zhang, Haipeng Yang and Yongfa Zhu

Page 2562



Current vs. potential curves for ZnWO₄ film treated at various temperatures: ((a) photo 500 °C; (b) photo 550 °C; (c) photo TiO₂; (d) dark 500 °C; (e) dark 550 °C; (f) dark TiO₂) in 0.5 M Na₂SO₄ solution pH 6.0, scan rate = 10 mV s^{-1} .

Synthesis, structure and luminescence property of two lanthanum phosphite hydrates: $La_2(H_2O)_x(HPO_3)_3$ (x = 1, 2)

Ding-Bang Xiong, Man-Rong Li, Wei Liu, Hao-Hong Chen, Xin-Xin Yang and Jing-Tai Zhao Page 2571



Two lanthanum phosphites, $La_2(H_2O)(HPO_3)_3$ (1) and $La_2(H_2O)_2(HPO_3)_3$ (2), were synthesized by modified hydrothermal methods and their crystal structures showed different arrangements of face-sharing dimers of La coordination polyhedron observed for the first time in rare-earth phosphites. The two Ce⁺³-doped compounds show intensive broad emission band around 340 nm under UV excitation.

Phase relations in $Na_x Cr_x Ti_{8-x}O_{16}$ at 1350 °C and crystal structure of hollandite-like $Na_2 Cr_2 Ti_6 O_{16}$ Yuichi Michiue

Page 2578



Difference Fourier map at the y = 0.5 section for Na₂Cr₂Ti₆O₁₆ with a structure model containing no Na ions.

 $(C_5H_{16}N_2) \cdot [Zn_3(HPO_3)_4] \cdot H_2O$: A new threedimensional zincophosphite with 12-membered ring channels and infinite edge shared 4-membered ring ladders Lei Wang, Hong Ding, Ying Hou, Linlin Zhu, Zhan Shi and Shouhua Feng *Page 2584*



View of the 3-D structure along the *a*-axis.

Preparation, luminescence and defect studies of Eu²⁺-activated strontium hexa-aluminate phosphor prepared via combustion method

Vijay Singh, T.K. Gundu Rao and Jun-Jie Zhu Page 2589



SEM image of SrAl₁₂O₁₉:Eu.

Crystal structures and magnetic properties of 6H-perovskite-type oxides $Ba_3MIr_2O_9$ (M=Mg, Ca, Sc, Ti, Zn, Sr, Zr, Cd and In)

Takeshi Sakamoto, Yoshihiro Doi and Yukio Hinatsu Page 2595



The schematic crystal structure of $Ba_3MIr_2O_9$. Among the title compounds, only $Ba_3M^{3+}Ir_2^{4.5+}O_9$ (M=Sc, In) show an antiferromagnetic transition at low temperatures.

Structural investigation of $La_{9.33}Si_6O_{26}$ - and $La_{9.AE}Si_6O_{26+\delta}$ -doped apatites-type lanthanum silicate (AE = Ba, Sr and Ca) by neutron powder diffraction S. Lambert, A. Vincent, E. Bruneton, S. Beaudet-Savignat, F. Guillet, B. Minot and F. Bouree *Page 2602*



Crystal structure of lanthanum silica apatite.

Ultrasonic synthesis of polyaniline nanotubes containing Fe_3O_4 nanoparticles

Xiaofeng Lu, Hui Mao, Danming Chao, Wanjin Zhang and Yen Wei *Page 2609*

FeCl₂ • 4H₂O + FeCl₃ • 6H₂O + NH₃ • H₂O + aniline dimer-COOH



Simplified schematic representation of the preparation of $PANI/Fe_3O_4$ composite nanotubes assisted by ultrasonic irradiation.

Na-Li-[V₃O₈] insertion electrodes: Structures and diffusion pathways

Michael Schindler, Frank C. Hawthorne, Malcolm A. Alexander, Rory A. Kutluoglu, Petre Mandaliev, Norman M. Halden and Roger H. Mitchell *Page 2616*



Bond-valence map for Li in $Na_{0.7}Li_{0.7}[V_3O_8]$. Contour lines representing the bond-valence sum of 1.0 vu are marked with thick black lines and indicate potential diffusion pathways of Li.

Structural, textural and photocatalytic properties of quantum-sized In₂S₃-sensitized Ti-MCM-41 prepared by ion-exchange and sulfidation methods

Shaohua Shen and Liejin Guo Page 2629



Proposed band energy diagram for $In_2S_3@\,Ti\text{-}MCM\text{-}41$ in an aqueous Na_2SO_3 solution (pH = 8.8).

Synthesis and optical characterizations of undoped and rare-earth-doped CaF_2 nanoparticles

A. Bensalah, M. Mortier, G. Patriarche, P. Gredin and D. Vivien

Page 2636



Transmission Electron Microscopy micrograph of CaF₂ nanoparticles synthesized by a reverse-micelle method.

$Ba_3Fe_2WO_{9-\delta}$: Effect of oxygen non-stoichiometry on structural and magnetic properties

S.A. Ivanov, S.-G. Eriksson, R. Tellgren, H. Rundlof, P. Nordblad and J. Eriksen *Page 2645*

C'm9



Magnetic structure of the oxygen-deficient perovskite $Ba_3Fe_2WO_{8.45}$.

System-pH-dependent supramolecular isomers of puckered three-dimensional layered hydrogen-bonded networks: Syntheses, characterization and fluorescent properties

Pang-Kuan Chen, Yun-Xia Che, Yu-Mei Li and Ji-Min Zheng

Page 2656



The schematic representation highlighting the pH-dependent formation in the synthesis processes of a pair of isomers.

Generation of WO₃–ZrO₂ catalysts from solid solutions of tungsten in zirconia

María A. Cortés-Jácome, Carlos Angeles-Chavez, Xim Bokhimi and J.A. Toledo-Antonio *Page 2663*



 WO_x -ZrO₂ catalysts were obtained by precipitating zirconium oxynitrate in presence of WO_4^- species. Initially, the W atoms remained inside the crystallite after annealing at 560 °C in a reduced oxidation state (W^{5+}), whereas, the sample annealed at 800 °C, the W atoms migrate from the bulk to the surface, forming a layer of W atoms on a ZrO₂ core, with the consequent oxidation to W^{6+} , producing patches of nanocrystalline WO₃ with dimension smaller than 3 nm.

Supercritical Propanol–Water Synthesis and Comprehensive Size Characterisation of Highly Crystalline anatase TiO₂ Nanoparticles

Peter Hald, Jacob Becker, Martin Bremholm, Jan S. Pedersen, Jacques Chevallier, Steen B. Iversen and Bo B. Iversen



The synthesis parameter space (T, P, concentration) for supercritical synthesis of TiO₂ in a propanol–water mixture has been explored, and the nanocrystalline products comprehensively characterized.

Structural transformations in the $Na_{4+x}VO(PO_4)_2$ vanadylphosphates

Roman V. Shpanchenko, Evgeny V. Dikarev, Andrev V. Mironov, Svetlana N. Mudretsova and

Evgeny V. Antipov





Bond valence calculations have been used to explain the charge redistribution between vanadium atoms in neighboring chains in the Na_{4+ δ}VO(PO₄)₂ structures.

Crystal structures and phase stability in pseudobinary $CaAl_{2-x}Zn_x$

Karin Söderberg, Magnus Boström, Yoshiki Kubota, Takeshi Nishimatsu, Rainer Niewa, Ulrich Häussermann, Yuri Grin and Osamu Terasaki *Page 2690*



The investigation of the pseudobinary system CaAl_{2-x}Zn_x yielded the structural sequence MgCu₂ (C15)–MgNi₂ (C36)–KHg₂ with increasing x. The structural change C15→C36 between two Laves phase structures is induced by the decrease in valence electron concentration. However, with increasing Zn content the system becomes increasingly polar and at some point favours the more open packed KHg₂ structure over a Laves phase structure.

Fabrication and optical properties of core–shell structured spherical SiO₂@GdVO₄:Eu³⁺ phosphors via sol–gel process

Guangzhi Li, Zhenling Wang, Min Yu, Zewei Quan and Jun Lin

Page 2698



Spherical SiO_2 particles have been coated with GdVO₄:Eu phosphor layers by a Pechini sol–gel process, which show the characteristic red emission of Eu³⁺.

Crystal structure, electronic structure and physical properties of the new low-valent thallium silicon telluride $Tl_6Si_2Te_6$ in comparison to $Tl_6Ge_2Te_6$

Abdeljalil Assoud, Navid Soheilnia and Holger Kleinke Page 2707



The isostructural tellurides $Tl_6Si_2Te_6$ and $Tl_6Ge_2Te_6$ contain $Si^{\rm III}$ and $Ge^{\rm III}$ in dimeric $[Si_2Te_6]^{6-}$ and $[Ge_2Te_6]^{6-}$ units, respectively. Both materials are black semiconductors with high Seebeck coefficients and reasonable electrical conductivities, despite their molecular character.

Electron-irradiation induced phase transformation in $La_{1/3}Zr_2(PO_4)_3$: La^{3+} displacement in a preserved NASICON framework

M.P. Crosnier-Lopez, M. Barre, F. Le Berre and J.L. Fourquet

Page 2714



Diffraction pattern of a crystallite of $La_{1/3}Zr_2(PO_4)_3$ showing the transformation under the electron beam (a) at the beginning and (b) at the end.

Thermodynamic properties of complex oxides in the La-Ni-O system

D.O. Bannikov and V.A. Cherepanov Page 2721



The crystal structure of La₄Ni₃O₁₀.

Rapid Communications

Low temperature synthesis of bilayer hydrated cesium cobalt oxide

Horng Y. Tang, Hsiao Y. Lin, Ming J. Wang, Ming Y. Liao, Fon C. Hsu, Boon H. Mok, Jean L. Liu, Michael T. Beasley, Hwo S. Sheu and Maw K. Wu *Page 2728*



BLH $Cs_{0.2}CoO_2\!\cdot\!0.63H_2O$ crystals grown from low temperature molten salt.

"Unusual" phase transitions in CeAlO₃ W.T. Fu and D.J.W. IJdo *Page 2732*



Temperature dependence of the octahedral tilting angles in CeAlO₃. The continuous line in rhombohedral phase region is the fit to the expression: $\phi = A(T_c-T)^{\beta}$ with fitted values of $T_c = 1371$ K, $\beta = 0.35$ and A = 0.52. Note that the lines that separate the *I4/mcm* and *Imma* phases and the *Imma* and $R\bar{3}c$ phases are not experimentally determined transition temperatures but for visualisation purpose.

NOTICE

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

Pressure-induced polymorphism in Al₃BC₃: A first-principles study

Jingyang Wang, Yanchun Zhou, Zhijun Lin and Ting Liao



Relative enthalpy of tetragonal phase with respect to hexagonal phase at various pressures. The pressure-induced phase transformation occurs at about 2 and 24 GPa for Mg_3BN_3 and Al_3BC_3 , respectively.