

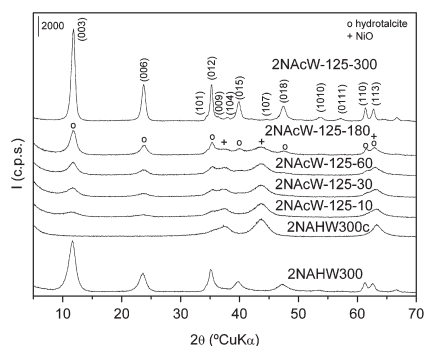
CONTENTS

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Regular Articles

Microwave-assisted reconstruction of Ni,Al hydroxalcalite-like compounds

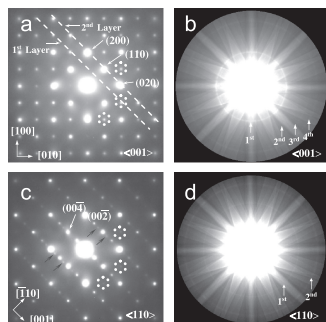
P. Benito, I. Guinea, F.M. Labajos and V. Rives
page 987



The microwave-assisted reconstruction of Ni,Al HTLcs with Ni/Al molar ratios 2/1 and 3/1 has been studied. Full recovering of the original layered structure is achieved in short periods of time for the 2/1 in the Na₂CO₃ solution, but more drastic conditions are necessary for the 3/1 samples and the reconstruction seems not to be completed. Only a partial reconstruction is observed in distilled water or NH₃ aqueous solution.

Electron microscopic studies of the antiferroelectric phase in Sr_{0.60}Ca_{0.40}TiO₃ ceramic

Shahid Anwar and N.P. Lalla
page 997

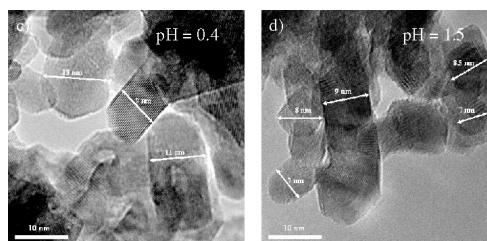


Selected area diffraction (SAD) and convergent beam electron diffraction (CBED) patterns taken along the (a,b) [001] and (c,d) [110] zones of the *Pbcm* phase from different domains. The occurrence of the FOLZ ring corresponding to 15.5 Å and the superlattice spots as indicated by black arrows confirming the existence of the cell-doubled antiferroelectric phase. Coexistence of the *Pbnm* and *Pbcm* phases across the transition, i.e. at room temperature, has been observed and attributed to the strain/disorder-induced broadening of the first-order antiferroelectric phase transition.

Regular Articles—Continued

Structure, microstructure, and size dependent catalytic properties of nanostructured ruthenium dioxide

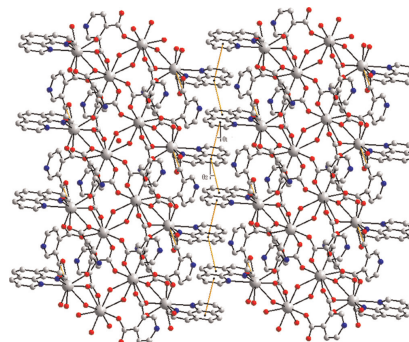
Pawel Nowakowski, Jean-Pierre Dallas, Sylvie Villain, Agnieszka Kopia and Jean-Raymond Gavarri
page 1005



Nanosized crystals of RuO₂ prepared by sol gel route, at pH = 0.4 and 1.5. Mean size values $\langle D \rangle$, respectively, 10 and 8 nm.

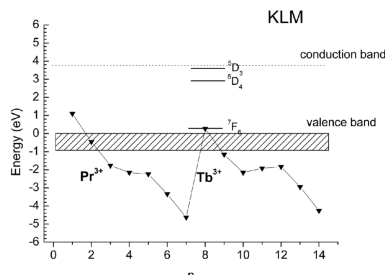
Synthesis, crystal structure and properties of two 1D nano-chain coordination polymers constructed by lanthanide with pyridine-3,4-dicarboxylic acid and 1,10-phenanthroline

Hui-Hua Song, Ya-Juan Li, You Song, Zhan-Gang Han and Fang Yang
page 1017



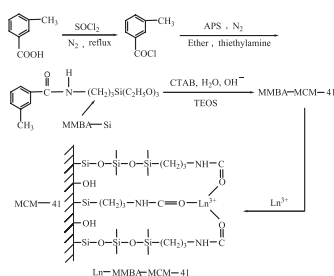
Two novel lanthanide coordination polymers [M₂(pydc)₃(phen)(H₂O)·H₂O]_n (M = Eu(1) and Tb(2), pydc = pyridine-3,4-dicarboxylate, phen = 1,10-phenanthroline) have been synthesized and characterized. Both compounds reveal a one-dimensional nano-chain, which is further assembled into a three-dimensional supramolecular network via π-π stacking interactions and hydrogen bonds. Their luminescent and magnetic properties have been investigated.

The excited state dynamics of $\text{KLa}(\text{MoO}_4)_2\text{Pr}^{3+}$: From a case study to the determination of the energy levels of rare earth impurities relative to the bandgap in oxidising host lattices
 Enrico Cavalli, Philippe Boutinaud, Marco Bettinelli and Pieter Dorenbos
 page 1025



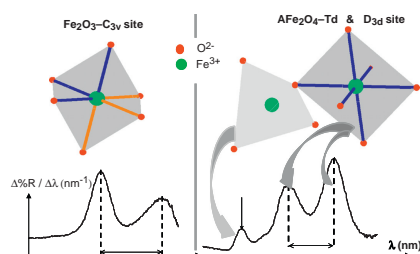
The study of the excited state dynamics of $\text{KLa}(\text{MoO}_4)_2$ single crystals doped with Pr^{3+} allows to determine the energies of the levels of the active ion relative to the valence and conduction bands of the host. This model has then been extended to the other rare earth ions on the basis of the systematic nature of the lanthanide energy levels properties.

Hybrid materials of MCM-41 functionalized by lanthanide (Tb^{3+} , Eu^{3+}) complexes of modified *meta*-methylbenzoic acid: Covalently bonded assembly and photoluminescence
 Ying Li and Bing Yan
 page 1032



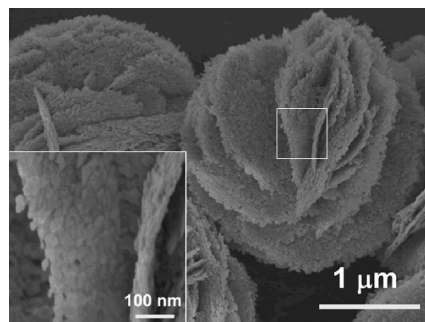
Novel organic-inorganic mesoporous luminescent materials were synthesized by linking lanthanide (Tb^{3+} , Eu^{3+}) complexes to covalently bond the functionalized ordered mesoporous MCM-41 with modified *meta*-methylbenzoic acid (MMBA)-Si by co-condensation of tetraethoxysilane (TEOS) in the presence of the cetyltrimethylammonium bromide (CTAB) surfactant as template.

Correlation between structural features and vis-NIR spectra of $\alpha\text{-Fe}_2\text{O}_3$ hematite and $A\text{Fe}_2\text{O}_4$ spinel oxides ($A = \text{Mg}, \text{Zn}$)
 N. Pailhé, A. Wattiaux, M. Gaudon and A. Demourgues
 page 1040



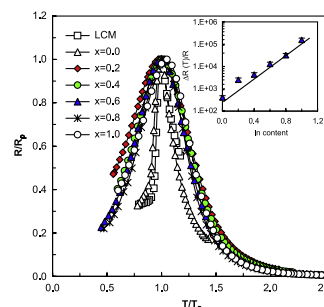
UV-visible-NIR reflectance of iron red pigments: MgFe_2O_4 , ZnFe_2O_4 spinels and Fe_2O_3 hematite, were analyzed in regard of their structural features: cationic distribution, geometry of the Fe^{3+} sites, ionic-covalence of the bonds.

Cooperative self-construction and enhanced optical absorption of nanoplates-assembled hierarchical Bi_2WO_6 flowers
 Shengwei Liu and Jianguo Yu
 page 1048



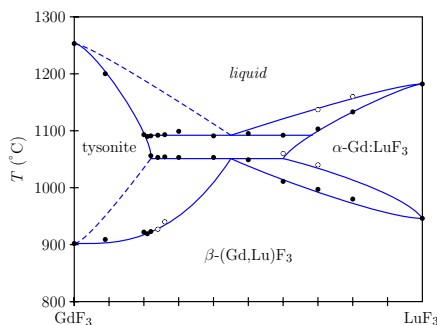
Bi_2WO_6 hierarchical multilayered flower-like assemblies are fabricated on a large scale by a simple hydrothermal method in the presence of polymeric poly(sodium 4-styrenesulfonate).

Synthesis, structure and electric studies for $\text{La}_{0.7}\text{A}_{0.3}\text{Mn}_{0.96}(\text{In}_x\text{Al}_{1-x})_{0.04}\text{O}_3$; $A = \text{Ca}$ and Sr perovskites
 M.F. Mostafa, S.S. Ata-Allah and H.S. Refai
 page 1056



The reduced resistivity $[R(T)/R(T_p)]$ vs. the reduced temperature $[T/T_p]$ of (Al and In) doped $\text{La}_{0.7}\text{Ca}_{0.3}\text{MnO}_3$ -manganites. The variation of the amplitude of the giant resistive peak $\Delta R(T)/R = [R(T_p) - R(T_{288K})]/R(T_{288K})$ with In content x (inset).

The phase diagram $\text{GdF}_3\text{-LuF}_3$
 I.M. Ranieri, S.L. Baldochi and D. Klimm
 page 1070



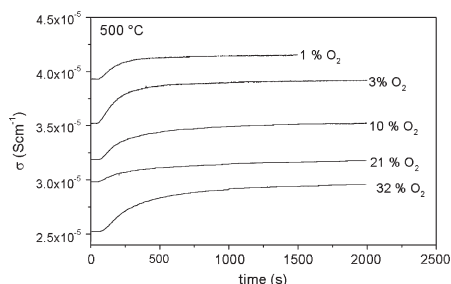
The phase diagram $\text{GdF}_3\text{-LuF}_3$, α , β mean high- T phase or low- T phase, respectively.

Continued

Oxygen partial pressure dependence of electrical conductivity in γ' -Bi₂MoO₆

C.M.C. Vera and R. Aragón

page 1075

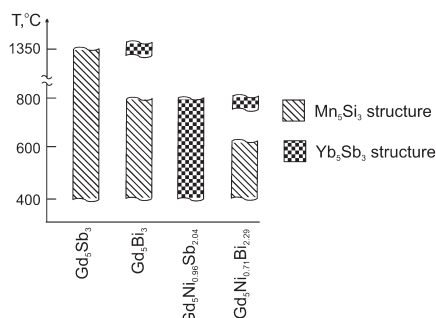


Temporal dependence of electrical conductivity at 500 °C for γ' -Bi₂MoO₆ at controlled partial pressures of oxygen.

Gd₅Ni_{0.96}Sb_{2.04} and Gd₅Ni_{0.71}Bi_{2.29}: Crystal structure, magnetic properties and magnetocaloric effect. Structural transformation and magnetic properties of hexagonal Gd₅Bi₃

Volodymyr Svitlyk, Fan Fei and Yuriy Mozharivskyy

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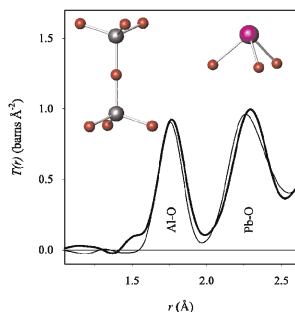


Ni substitution of Sb in Gd₅Sb₃ and Gd₅Bi₃ leads to the formation of the orthorhombic Yb₅Sb₃-type structure for Gd₅Ni_{0.96}Sb_{2.04} and stabilizes the orthorhombic bismuthide Gd₅Ni_{0.71}Bi_{2.29} to lower temperatures. Magnetic behavior and magnetocaloric effect was studied for hexagonal Mn₅Si₃-type Gd₅Bi₃, and orthorhombic Gd₅Ni_{0.96}Sb_{2.04} and Gd₅Ni_{0.71}Bi_{2.29}.

Local structure and disorder in crystalline Pb₉Al₈O₂₁

Alex C. Hannon, Emma R. Barney, Diane Holland and Kevin S. Knight

page 1087

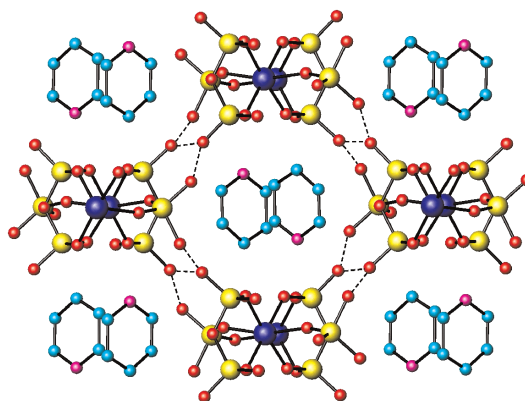


Combined neutron powder diffraction and total scattering, and ²⁷Al NMR on crystalline Pb₉Al₈O₂₁ shows it to be a non-stoichiometric compound with vacancies due to PbO volatilisation. A detailed consideration of the thermal and static disorder is given, showing that glass and crystal phases have very similar disorder at short range.

Supramolecular open-framework based on 1-D iron phosphate–diphosphate chains assembled through hydrogen bonding

Miguel A. Salvadó, Pilar Pertierra, Camino Trobajo and José R. García

page 1103

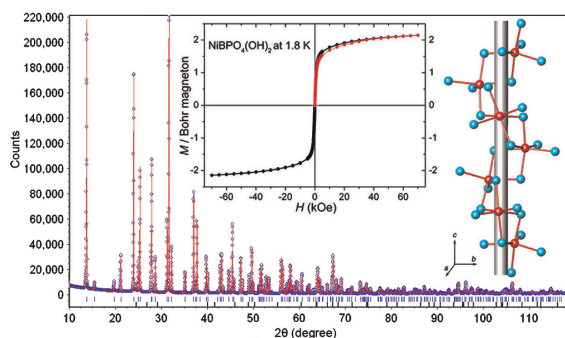


The low temperature hydrothermal synthesis offers many possibilities in the preparation of new materials with mixed octahedral–tetrahedral open-frameworks. Fe(H₂PO₄)(H₂P₂O₇)·C₅H₅N is constituted by linear chains of FeO₆ octahedra joined through of both dihydrogenphosphate and dihydrogendiphosphate bridges, interconnected by hydrogen bonds, originating channels where the pyridine molecules are located.

Chirality and ferromagnetism in NiBPO₄(OH)₂ containing helix edge-sharing NiO₆ chains

Tao Yang, Jing Ju, Fuhui Liao, Juns Sasaki, Naoki Toyota and Jianhua Lin

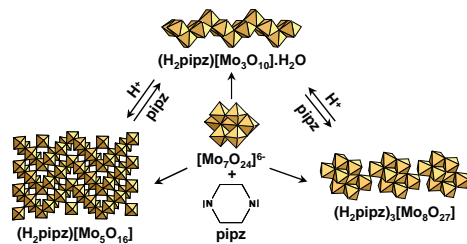
page 1110



Two isotopic borophosphates MBPO₄(OH)₂ (M = Mg, Ni) have been hydrothermally synthesized and structurally characterized by powder X-ray diffraction in the space group P3₁21. Nickel (or magnesium) atoms are octahedrally coordinated, which further share edges forming NiO₆ chains around the three-fold screw-axis. Magnetic investigation of NiBPO₄(OH)₂ shows that it is a quasi-one-dimensional magnet, where the intra- and inter-chain interactions are proved to be both ferromagnetic, and a long-range ordering is established below 2.2 K.

Reinvestigation of hybrid organic–inorganic materials based on molybdate and piperazininium cations: Influence of the synthesis conditions on the chemical composition and characterizations of the photochromic properties

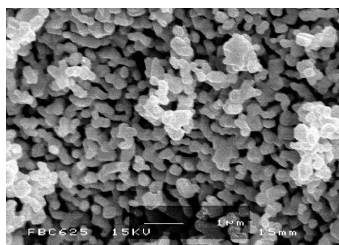
Violaine Coué, Rémi Dessapt, Martine Bujoli-Doeuff, Michel Evain and Stéphane Jobic
page 1116



Three organic–inorganic hybrid materials have been prepared from the investigations of the $[\text{Mo}_7\text{O}_{24}]^{6-}$ /piperazine system in hydrothermal conditions. The role of the pH on the stabilization of the different polyoxomolybdate blocks in the materials i.e. $\frac{1}{\infty}[\text{Mo}_3\text{O}_{10}]^{2-}$ and $\frac{1}{\infty}[\text{Mo}_8\text{O}_{27}]^{6-}$ chains and $\frac{2}{\infty}[\text{Mo}_5\text{O}_{16}]^{2-}$ layer has been investigated.

Direct syntheses of $\text{La}_{n+1}\text{Ni}_n\text{O}_{3n+1}$ phases ($n = 1, 2, 3$ and ∞) from nanosized co-crystallites

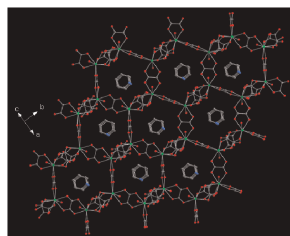
Xiaole Weng, Paul Boldrin, Isaac Abrahams, Stephen J. Skinner, Suela Kellici and Jawwad A. Darr
page 1123



Scanning electron micrograph of $\text{La}_4\text{Ni}_3\text{O}_{10}$ (bar = 1 μm) made by a single heat treatment at 1075 $^\circ\text{C}$ in air for 12 h of a 4:3 La:Ni ratio co-crystallite mixture of the metal hydroxides.

Hydrothermal synthesis and characteristics of 3-D hydrated bismuth oxalate coordination polymers with open-channel structure

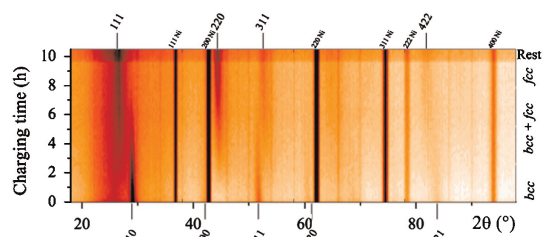
Xinxiang Chen, Yanning Cao, Hanhui Zhang, Yiping Chen, Xuehuan Chen and Xiaochuan Chai
page 1133



Two novel 3-D extended porous coordination polymers have been synthesized by hydrothermal method. Both compounds are 3-D open-framework structures with a 6^6 uniform net, which consist of honeycomb-like layers connected to each other by oxalate units. While different guest molecules fill in their cavities of honeycomb-like layers. Study of ultrasonic treatment on **2** indicates the replacement of NH_4^+ by K^+ on potassium ion exchange.

In situ neutron diffraction study on Pd-doped $\text{Mg}_{0.65}\text{Sc}_{0.35}$ electrode material

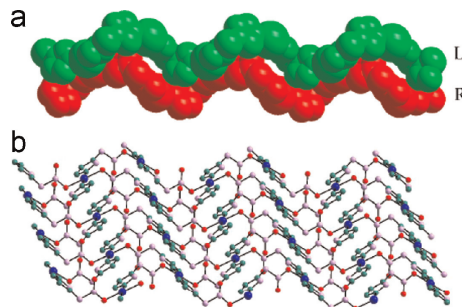
W.P. Kalisvaart, M. Latroche, F. Cuevas and P.H.L. Notten
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2D projection of the neutron diffraction pattern intensities as function of time during electrochemical charge of Pd-doped $\text{Mg}_{0.65}\text{Sc}_{0.35}$ active material showing the progressive transformation from bcc to fcc.

Syntheses, crystal structure and properties of two novel coordination polymers with the flexible tetrazole-1-acetic acid (Htza)

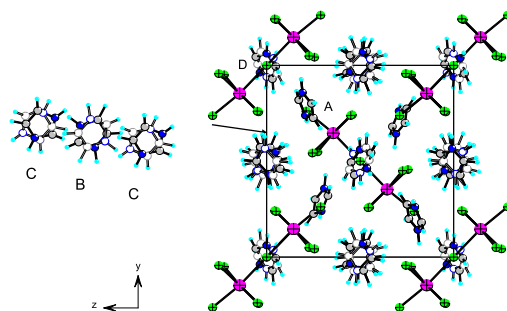
Wen-Wen Dong, Jun Zhao and Li Xu
page 1149



Two novel coordination polymers, $[\text{Ag}(\text{tza})]_{\infty}$ (**1**) and $[\text{Cu}(\text{tza})_2]_{\infty}$ (**2**) have been prepared and characterized. Compound **1** features extended double-stranded helical chains. Compound **2** features undulated layered structure with hourglass-shaped $[\text{Cu}_4(\text{tza})_4]$ as subunits with the weak ferromagnetic interactions between Cu(II) ions.

Structural characterization and ferroelectric ordering in $(\text{C}_3\text{N}_2\text{H}_5)_5\text{Sb}_2\text{Br}_{11}$

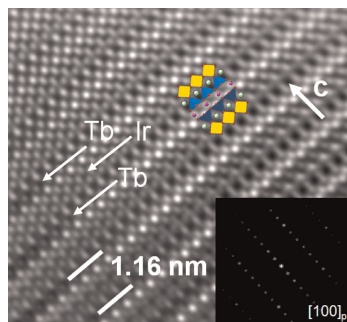
A. Piecha, A. Pietraszko, G. Bator and R. Jakubas
page 1155



Crystal packing down the a -axis in $(\text{C}_3\text{N}_2\text{H}_5)_5\text{Sb}_2\text{Br}_{11}$ in plane **II** at 155 K.

IrSr₂TbCu₂O₈, a high-pressure metamagnetic cuprate: Structure, microstructure and properties

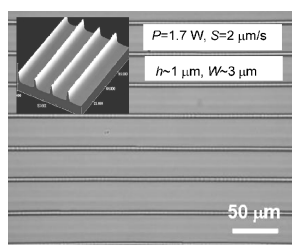
A.J. Dos santos-García, J. van Duijn, R. Saéz-Puche, G. Heymann, H. Huppertz and M.A. Alario-Franco
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Reconstructed image from the SAED of the long *c* tetragonal axis ($3a_p$) of an IrSr₂TbCu₂O₈ crystal. A unit cell picture is included for comparison.

Spatially selected synthesis of LaF₃ and Er³⁺-doped CaF₂ crystals in oxyfluoride glasses by laser-induced crystallization

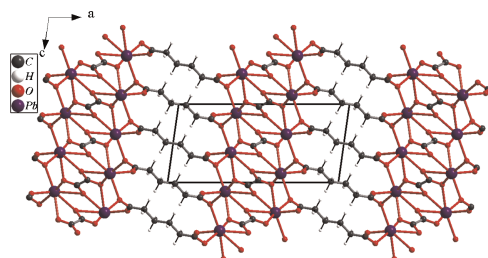
M. Kusatsugu, M. Kanno, T. Honma and T. Komatsu
page 1176



This figure shows the polarization optical and confocal scanning laser micrographs for lines obtained by laser irradiations with a laser power of $P=1.7$ W and a scanning speed of $S=2$ μm/s in an oxyfluoride glass. It is proposed that the line consists of the composite of CaF₂ nanocrystals and oxide glassy phase. This is the first demonstration on the patterning of fluoride crystals in glass by laser irradiations.

Hybrid structures formed by homo- and heteroleptic aliphatic dicarboxylates of lead with 2-D inorganic connectivity

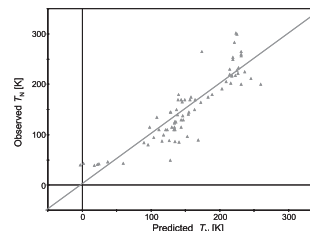
A. Thirumurugan and C.N.R. Rao
page 1184



Three homoleptic and two heteroleptic three-dimensional lead aliphatic dicarboxylates along with a novel two-dimensional lead nitrate-oxalate with hybrid structures involving Pb–O–Pb linkages have been synthesized and characterized. In all these dicarboxylates, there is two-dimensional inorganic connectivity. The lead (II) cation has hemi- or holo-directed coordination geometry.

Multivariate data analysis approach to understand magnetic properties of perovskite manganese oxides

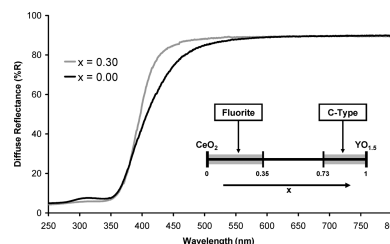
N. Imamura, T. Mizoguchi, H. Yamauchi and M. Karppinen
page 1195



Statistical multivariate data analysis techniques are applied to detect structure-property relations in antiferromagnetic (AFM) and ferromagnetic (FM) manganese perovskites. For AFM compounds, *partial least squares projections to latent structures* analysis predict the magnitude of the Néel temperature on the bases of structural parameters only. Moreover, AFM and FM compounds are well separated by means of so-called *partial least squares discriminant analysis* method.

Powder preparation and UV absorption properties of selected compositions in the CeO₂–Y₂O₃ system

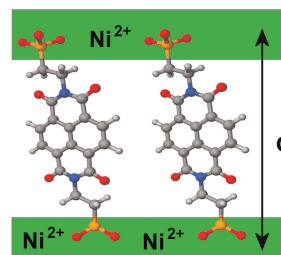
Franck Tessier, François Cheviré, Francisco Muñoz, Odile Merdrignac-Conanec, Roger Marchand, Michel Bouchard and Christophe Colbeau-Justin
page 1204



Comparison between diffuse reflectance spectra of ceria ($x=0$) and yttrium modified ceria ($x=0.3$).

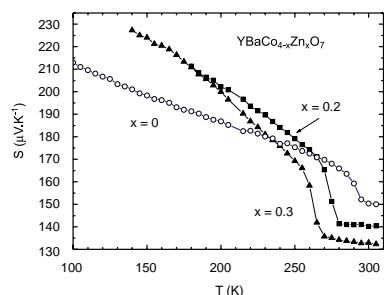
Synthesis and characterization of a new layered organic–inorganic hybrid nickel(II) 1,4:5,8-naphthalenediimide *bis*-phosphonate, exhibiting canted antiferromagnetism, with $T_c \sim 21$ K

Elvira M. Bauer, Carlo Bellitto, Carlos J. Gómez García and Guido Righini
page 1213



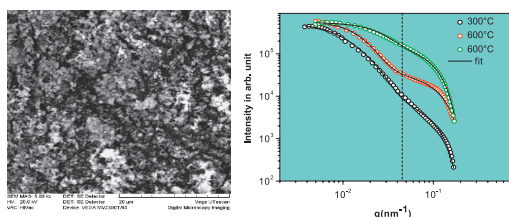
A new layered hybrid organic–inorganic Ni(II) *N,N'*-*bis*(2-phosphonoethyl)-naphthalene 1,4:5,8 tetracarboxydiimide complex has been synthesized and characterized. Magnetic measurements as a function of temperature and at different fields show that the compound is magnetically ordered below $T_c \sim 21$ K.

Impact of metal substitutions for cobalt in YBaCo_4O_7
 A. Maignan, V. Caignaert, V. Pralong, D. Pelloquin and
 S. Hébert
page 1220



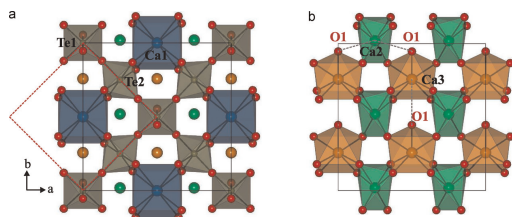
The temperature characteristic of the structural transition in YBaCo_4O_7 , indicated by an abrupt jump of the Seebeck coefficient, decreases as Zn^{2+} is substituted for cobalt. In contrast, Al^{3+} or Ga^{3+} substitutions suppress this structural transition.

Effect of heat treatment on pore structure in nano-crystalline NiO: A small angle neutron scattering study
 J. Bahadur, D. Sen, S. Mazumder and S. Ramanathan
page 1227



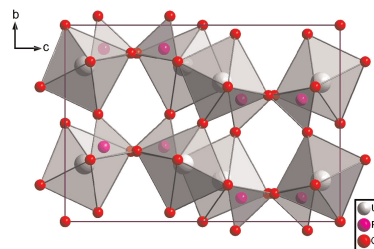
SEM micrograph shows the microstructure of the nano-crystalline NiO. An average agglomerate size of $\sim 1 \mu\text{m}$ is evident from SEM and LS.SANS profiles for the samples heat treated at 300, 600 and 900 $^\circ\text{C}$, respectively, are shown. A significant variation in the profile shape due to the modification in the intra-agglomerate pore structure under heat treatment is visible.

Chiolite-like $\text{Ca}_5\text{Te}_3\text{O}_{14}$: An X-ray and neutron diffraction study
 W.T. Fu and D.J.W. IJdo
page 1236



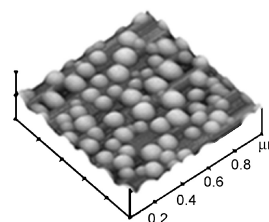
The structure of $\text{Ca}_5\text{Te}_3\text{O}_{14}$ around $z=0$ (a) and 0.25 (b), respectively. The dimension of the unit cell is drawn in full line and that of the sub-cell in dashed line. In (b) the relatively too long Ca2–O1 and Ca3–O1 bond distances are also shown in dashed line.

Pressure induced phase transformation in $\text{U}_2\text{O}(\text{PO}_4)_2$
 A.K. Mishra, Chitra Murli, A. Singhal and
 Surinder M. Sharma
page 1240



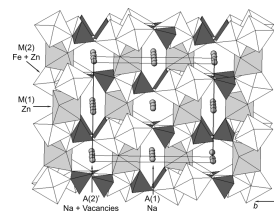
The high pressure behavior of $\text{U}_2\text{O}(\text{PO}_4)_2$ has been investigated with the help of Raman scattering and X-ray diffraction measurements up to ~ 14 and 6.5 GPa , respectively. The observed changes in the Raman spectra as well as the X-ray diffraction patterns suggest that $\text{U}_2\text{O}(\text{PO}_4)_2$ undergoes a phase transition at $\sim 6 \text{ GPa}$ to a mixture of a disordered ambient pressure phase and a new high pressure phase. The new phase resembles the triclinic mixed-valence phase of uranium orthophosphate ($\text{U}(\text{UO}_2)(\text{PO}_4)_2$). On release of pressure the initial phase is not retrieved.

Shape controlled synthesis of CaMoO_4 thin films and their photoluminescence property
 Ana Paula de Azevedo Marques, Valeria M. Longo,
 Dulce M.A. de Melo, Paulo S. Pizani, Edson R. Leite,
 José Arana Varela and Elson Longo
page 1249



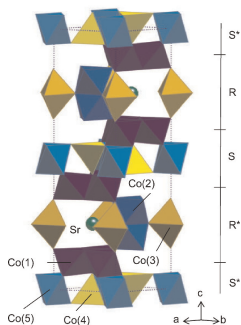
CaMoO_4 thin films were prepared by the complex polymerization method (CPM). The films were annealed at different temperatures and time in a conventional resistive furnace and in a microwave oven. A strong photoluminescence emission was observed in the disordered thin films and was attributed to complex cluster vacancies. The experimental results were confirmed by high level first principle calculations.

Crystal chemistry of the divalent cation in alluaudite-type phosphates: A structural and infrared spectral study of the $\text{Na}_{1.5}(\text{Mn}_{1-x}\text{M}^{2+}_x)_1.5\text{Fe}_{1.5}(\text{PO}_4)_3$ solid solutions ($x=0$ to 1 , $\text{M}^{2+} = \text{Cd}^{2+}, \text{Zn}^{2+}$)
 Frédéric Hatert
page 1258



The crystal structure of $\text{Na}_{1.5}\text{Zn}_{1.5}\text{Fe}_{1.5}^{3+}(\text{PO}_4)_3$.

High pressure synthesis and structure of a new magnetoplumbite-type cobalt oxide $\text{SrCo}_{12}\text{O}_{19}$
Shintaro Ishiwata, Ichiro Terasaki, Masaki Azuma and Mikio Takano
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A new magnetoplumbite-type hexagonal cobalt oxide, $\text{SrCo}_{12}\text{O}_{19}$, has been synthesized by a high-pressure technique. Bond-valence calculations based on a single crystal X-ray structure refinement show a rather wide charge distribution for Co sites from +2.15 (Co(4)) to +3.50 (Co(1)).

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